dodecyl benzoate

Other names: Benzoic acid, dodecyl ester
Inchi: InChI=1S/C19H30O2/c1-2-3-4-5-6-7-8-9-10-14-17-21-19(20)18-15-12-11-13-16-18/h11-1
InchiKey: DLAHAXOYRFRPFQ-UHFFFAOYSA-N
Formula: C19H30O2
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 290.44
CAS: 2915-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-12.41	kJ/mol	Joback Method
hf	-443.76	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	69.32	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.764		Crippen Method
mcvol	262.250	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2173.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2163.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2173.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2181.00		NIST Webbook
rinpol	2168.00		NIST Webbook
ripol	2710.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2683.00		NIST Webbook
ripol	2681.00		NIST Webbook

ripol	2709.00		NIST Webbook
ripol	2694.00		NIST Webbook
ripol	2681.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2708.00		NIST Webbook
ripol	2677.00		NIST Webbook
ripol	2691.00		NIST Webbook
ripol	2709.00		NIST Webbook
ripol	2694.00		NIST Webbook
tb	737.09	K	Joback Method
tc	928.11	K	Joback Method
tf	402.47	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.05	J/mol×K	737.09	Joback Method
cpg	786.09	J/mol×K	768.93	Joback Method
cpg	803.11	J/mol×K	800.76	Joback Method
cpg	819.14	J/mol×K	832.60	Joback Method
cpg	834.22	J/mol×K	864.43	Joback Method
cpg	848.38	J/mol×K	896.27	Joback Method
cpg	861.65	J/mol×K	928.11	Joback Method
dvisc	0.0014187	Pa×s	402.47	Joback Method
dvisc	0.0006659	Pa×s	458.24	Joback Method
dvisc	0.0003683	Pa×s	514.01	Joback Method
dvisc	0.0002288	Pa×s	569.78	Joback Method
dvisc	0.0001547	Pa×s	625.55	Joback Method
dvisc	0.0001115	Pa×s	681.32	Joback Method
dvisc	0.0000845	Pa×s	737.09	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2915722&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume