Benzoic acid, nonadecyl ester

Inchi: InChI=1S/C26H44O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-24-28-26(27)25-22
InchiKey: UFFZSCVAOGUEKB-UHFFFAOYSA-N
Formula: C26H44O2
SMILES: CCCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1
Mol. weight [g/mol]: 388.63

Physical Properties

Property code	Value	Unit	Source
gf	46.53	kJ/mol	Joback Method
hf	-588.24	kJ/mol	Joback Method
hfus	59.92	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	8.495		Crippen Method
mcvol	360.880	ml/mol	McGowan Method
pc	898.02	kPa	Joback Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	897.25	K	Joback Method
tc	1098.93	K	Joback Method
tf	481.36	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1192.71	J/mol×K	897.25	Joback Method
cpg	1212.65	J/mol×K	930.86	Joback Method
cpg	1231.30	J/mol×K	964.48	Joback Method
cpg	1248.73	J/mol×K	998.09	Joback Method
cpg	1265.00	J/mol×K	1031.70	Joback Method
cpg	1280.17	J/mol×K	1065.31	Joback Method
cpg	1294.30	J/mol×K	1098.93	Joback Method
dvisc	0.0006695	Pa×s	481.36	Joback Method

dvisc	0.0002930	Pa×s	550.67	Joback Method
dvisc	0.0001542	Pa×s	619.99	Joback Method
dvisc	0.0000924	Pa×s	689.30	Joback Method
dvisc	0.0000608	Pa×s	758.62	Joback Method
dvisc	0.0000429	Pa×s	827.93	Joback Method
dvisc	0.0000319	Pa×s	897.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340232&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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