Dodecanoic acid, 2-phenylethyl ester

Other names: 2-Phenylethyl laurate
2-Phenylethyl dodecanoate
Inchi: InChI=1S/C20H32O2/c1-2-3-4-5-6-7-8-9-13-16-20(21)22-18-17-19-14-11-10-12-15-19/h1
InchiKey: WAKJZNSYKIRWFX-UHFFFAOYSA-N
Formula: C20H32O2
SMILES: CCCCCCCCCCCC(=O)OCCc1ccccc1
Mol. weight [g/mol]: 304.47
CAS: 6309-54-2

Physical Properties

Property code	Value	Unit	Source
gf	-3.99	kJ/mol	Joback Method
hf	-464.40	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	71.55	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.693		Crippen Method
mcvol	276.340	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	2264.20		NIST Webbook
rinpol	2264.20		NIST Webbook
tb	759.97	K	Joback Method
tc	950.54	K	Joback Method
tf	413.74	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.21	J/mol×K	759.97	Joback Method
cpg	844.50	J/mol×K	791.73	Joback Method
cpg	861.73	J/mol×K	823.49	Joback Method
cpg	877.96	J/mol×K	855.25	Joback Method
cpg	893.22	J/mol×K	887.02	Joback Method

cpg	907.53	J/mol×K	918.78	Joback Method
cpg	920.95	J/mol×K	950.54	Joback Method
dvisc	0.0012920	Pa×s	413.74	Joback Method
dvisc	0.0005995	Pa×s	471.44	Joback Method
dvisc	0.0003289	Pa×s	529.15	Joback Method
dvisc	0.0002031	Pa×s	586.86	Joback Method
dvisc	0.0001367	Pa×s	644.56	Joback Method
dvisc	0.0000982	Pa×s	702.27	Joback Method
dvisc	0.0000742	Pa×s	759.97	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6309542&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