Octadecanoic acid, phenylmethyl ester

Other names: Benzyl stearate
Inchi: InChI=1S/C25H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-22-25(26)27-23-24-20-17
InchiKey: BPSLVNCMKDXZPC-UHFFFAOYSA-N
Formula: C25H42O2
SMILES: CCCCCCCCCCCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]: 374.60
CAS: 5531-65-7

Physical Properties

Property code	Value	Unit	Source
gf	38.11	kJ/mol	Joback Method
hf	-567.60	kJ/mol	Joback Method
hfus	57.33	kJ/mol	Joback Method
hvap	82.68	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	7.991		Crippen Method
mcvol	346.790	ml/mol	McGowan Method
pc	952.01	kPa	Joback Method
rinpol	2727.00		NIST Webbook
rinpol	2794.30		NIST Webbook
rinpol	2794.30		NIST Webbook
tb	874.37	K	Joback Method
tc	1072.27	K	Joback Method
tf	470.09	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.86	J/mol×K	874.37	Joback Method
cpg	1216.10	J/mol×K	1039.29	Joback Method
cpg	1201.09	J/mol×K	1006.30	Joback Method
cpg	1185.01	J/mol×K	973.32	Joback Method
cpg	1167.82	J/mol×K	940.34	Joback Method

cpg	1149.45	J/mol×K	907.35	Joback Method
cpg	1230.10	J/mol×K	1072.27	Joback Method
dvisc	0.0000370	Pa×s	874.37	Joback Method
dvisc	0.0000495	Pa×s	806.99	Joback Method
dvisc	0.0000700	Pa×s	739.61	Joback Method
dvisc	0.0001061	Pa×s	672.23	Joback Method
dvisc	0.0001764	Pa×s	604.85	Joback Method
dvisc	0.0003330	Pa×s	537.47	Joback Method
dvisc	0.0007543	Pa×s	470.09	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5531657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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