Heptadecanoic acid, phenylmethyl ester

Other names:	Benzyl heptadecanoate
Inchi:	InChI=1S/C24H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-21-24(25)26-22-23-19-16-15
InchiKey:	XFIKDNCHPGLFLR-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCCCCCCCCCCC(=O)OCc1ccccc1
Mol. weight [g/mol]:	360.57
CAS:	74978-19-1

Physical Properties

Property code	Value	Unit	Source
gf	29.69	kJ/mol	Joback Method
hf	-546.96	kJ/mol	Joback Method
hfus	54.74	kJ/mol	Joback Method
hvap	80.45	kJ/mol	Joback Method
log10ws	-8.33		Crippen Method
logp	7.601		Crippen Method
mcvol	332.700	ml/mol	McGowan Method
pc	1011.02	kPa	Joback Method
tb	851.49	K	Joback Method
tc	1046.47	K	Joback Method
tf	458.82	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1067.64	J/mol×K	851.49	Joback Method
cpg	1086.92	J/mol×K	883.99	Joback Method
cpg	1105.03	J/mol×K	916.48	Joback Method
cpg	1122.01	J/mol×K	948.98	Joback Method
cpg	1137.91	J/mol×K	981.47	Joback Method
cpg	1152.77	J/mol×K	1013.97	Joback Method
cpg	1166.66	J/mol×K	1046.47	Joback Method
dvisc	0.0008470	Pa×s	458.82	Joback Method

dvisc	0.0003773	Pa×s	524.26	Joback Method
dvisc	0.0002011	Pa×s	589.71	Joback Method
dvisc	0.0001216	Pa×s	655.15	Joback Method
dvisc	0.0000805	Pa×s	720.60	Joback Method
dvisc	0.0000571	Pa×s	786.04	Joback Method
dvisc	0.0000427	Pa×s	851.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74978191&Units=SI

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

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