Heptadecanoic acid, hexyl ester

Other names: Hexyl heptadecanoate
Inchi: InChI=1S/C23H46O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-21-23(24)25-22-20-8-6
InchiKey: JQIUFPPAGDWAEH-UHFFFAOYSA-N
Formula: C23H46O2
SMILES: CCCCCCCCCCCCCCCCC(=O)OCCCCCC
Mol. weight [g/mol]: 354.61

Physical Properties

Property code	Value	Unit	Source
gf	-91.14	kJ/mol	Joback Method
hf	-762.85	kJ/mol	Joback Method
hfus	58.11	kJ/mol	Joback Method
hvap	75.95	kJ/mol	Joback Method
log10ws	-8.31		Crippen Method
logp	7.981		Crippen Method
mcvol	342.370	ml/mol	McGowan Method
pc	875.32	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	801.93	K	Joback Method
tc	982.34	K	Joback Method
tf	421.13	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1093.53	J/mol×K	801.93	Joback Method
cpg	1114.64	J/mol×K	832.00	Joback Method
cpg	1134.65	J/mol×K	862.07	Joback Method
cpg	1153.61	J/mol×K	892.14	Joback Method
cpg	1171.55	J/mol×K	922.21	Joback Method
cpg	1188.50	J/mol×K	952.27	Joback Method
cpg	1204.49	J/mol×K	982.34	Joback Method

dvisc	0.0011936	Pa×s	421.13	Joback Method
dvisc	0.0004928	Pa×s	484.60	Joback Method
dvisc	0.0002498	Pa×s	548.06	Joback Method
dvisc	0.0001457	Pa×s	611.53	Joback Method
dvisc	0.0000941	Pa×s	675.00	Joback Method
dvisc	0.0000655	Pa×s	738.46	Joback Method
dvisc	0.0000483	Pa×s	801.93	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=U405202&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume