

2-Heptenoic acid, octadecyl ester

Inchi: InChI=1S/C25H48O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-22-24-27-25(26)23-
InchiKey: PZRJMITWENUEBQ-XTQSDGFTSA-N
Formula: C25H48O2
SMILES: CCCCC=CC(=O)OCCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 380.65

Physical Properties

Property code	Value	Unit	Source
gf	5.92	kJ/mol	Joback Method
hf	-686.91	kJ/mol	Joback Method
hfus	63.49	kJ/mol	Joback Method
hvap	80.36	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	8.537		Crippen Method
mcvol	366.250	ml/mol	McGowan Method
pc	807.08	kPa	Joback Method
rinpol	2761.00		NIST Webbook
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tb	851.85	K	Joback Method
tc	1042.93	K	Joback Method
tf	438.59	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.11	J/mol×K	851.85	Joback Method
cpg	1216.70	J/mol×K	883.70	Joback Method
cpg	1237.13	J/mol×K	915.54	Joback Method
cpg	1256.44	J/mol×K	947.39	Joback Method
cpg	1274.69	J/mol×K	979.23	Joback Method
cpg	1291.93	J/mol×K	1011.08	Joback Method
cpg	1308.21	J/mol×K	1042.93	Joback Method
dvisc	0.0008783	Pa×s	438.59	Joback Method

dvisc	0.0003461	Pa×s	507.47	Joback Method
dvisc	0.0001704	Pa×s	576.34	Joback Method
dvisc	0.0000976	Pa×s	645.22	Joback Method
dvisc	0.0000622	Pa×s	714.10	Joback Method
dvisc	0.0000430	Pa×s	782.97	Joback Method
dvisc	0.0000315	Pa×s	851.85	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=U406103&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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