

3-Octenoic acid, heptadecyl ester

Inchi:	InChI=1S/C25H48O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-20-22-24-27-25(26)23-21-
InchiKey:	ZRRAAYLJGBVKLA-XUTLUUPISA-N
Formula:	C25H48O2
SMILES:	CCCCC=CCC(=O)OCCCCCCCCCCCCCCCCCC
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
rinsol	2685.00		NIST Webbook
tb	851.85	K	Joback Method
tc	1042.93	K	Joback Method
tf	438.59	K	Joback Method
vc	1.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1195.11	J/molxK	851.85	Joback Method
cpg	1216.70	J/molxK	883.70	Joback Method
cpg	1237.13	J/molxK	915.54	Joback Method
cpg	1256.44	J/molxK	947.39	Joback Method
cpg	1274.69	J/molxK	979.23	Joback Method
cpg	1291.93	J/molxK	1011.08	Joback Method
cpg	1308.21	J/molxK	1042.93	Joback Method
dvisc	0.0008783	Paxs	438.59	Joback Method
dvisc	0.0003461	Paxs	507.47	Joback Method

dvisc	0.0001704	Paxs	576.34	Joback Method
dvisc	0.0000976	Paxs	645.22	Joback Method
dvisc	0.0000622	Paxs	714.10	Joback Method
dvisc	0.0000430	Paxs	782.97	Joback Method
dvisc	0.0000315	Paxs	851.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406136&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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