2-Heptenoic acid, heptadecyl ester

Inchi: InChI=1S/C24H46O2/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-21-23-26-24(25)22-20-
InchiKey: RFYKKCCZKLVYTM-LSDHQDQOSA-N
Formula: C24H46O2
SMILES: CCCCC=CC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 366.62

Physical Properties

Property code	Value	Unit	Source
gf	-2.50	kJ/mol	Joback Method
hf	-666.27	kJ/mol	Joback Method
hfus	60.90	kJ/mol	Joback Method
hvap	78.13	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	8.147		Crippen Method
mcvol	352.160	ml/mol	McGowan Method
pc	852.97	kPa	Joback Method
rinpol	2662.00		NIST Webbook
rinpol	2662.00		NIST Webbook
tb	828.97	K	Joback Method
tc	1015.16	K	Joback Method
tf	427.32	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1131.61	J/mol×K	828.97	Joback Method
cpg	1152.63	J/mol×K	860.00	Joback Method
cpg	1172.54	J/mol×K	891.03	Joback Method
cpg	1191.40	J/mol×K	922.06	Joback Method
cpg	1209.26	J/mol×K	953.09	Joback Method
cpg	1226.16	J/mol×K	984.13	Joback Method
cpg	1242.15	J/mol×K	1015.16	Joback Method
dvisc	0.0009923	Pa×s	427.32	Joback Method

dvisc	0.0003939	Pa×s	494.26	Joback Method
dvisc	0.0001949	Pa×s	561.20	Joback Method
dvisc	0.0001121	Pa×s	628.14	Joback Method
dvisc	0.0000717	Pa×s	695.09	Joback Method
dvisc	0.0000496	Pa×s	762.03	Joback Method
dvisc	0.0000364	Pa×s	828.97	Joback Method

Sources

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=U406102&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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