Tetradecyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C19H36O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-21-19(20)18(3)5-2/h5H,4,6-
InchiKey: WLDMOCSBNXQITG-BLLMUTORSA-N
Formula: C19H36O2
SMILES: CC=C(C)C(=O)OCCCCCCCCCCCCCC
Mol. weight [g/mol]: 296.49

Physical Properties

Property code	Value	Unit	Source
gf	-53.15	kJ/mol	Joback Method
hf	-572.86	kJ/mol	Joback Method
hfus	46.65	kJ/mol	Joback Method
hvap	67.08	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.197		Crippen Method
mcvol	281.710	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2132.00		NIST Webbook
tb	714.45	K	Joback Method
tc	889.11	K	Joback Method
tf	357.01	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.85	J/mol×K	714.45	Joback Method
cpg	844.72	J/mol×K	743.56	Joback Method
cpg	862.70	J/mol×K	772.67	Joback Method
cpg	879.84	J/mol×K	801.78	Joback Method
cpg	896.15	J/mol×K	830.89	Joback Method
cpg	911.68	J/mol×K	860.00	Joback Method
cpg	926.44	J/mol×K	889.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373709&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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