Undecyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C16H30O2/c1-4-6-7-8-9-10-11-12-13-14-18-16(17)15(3)5-2/h5H,4,6-14H2,1-3
InchiKey: XZQGJOXZQNBUQA-PJQLUOCWSA-N
Formula: C16H30O2
SMILES: CC=C(C)C(=O)OCCCCCCCCCCC
Mol. weight [g/mol]: 254.41

Physical Properties

Property code	Value	Unit	Source
gf	-78.41	kJ/mol	Joback Method
hf	-510.94	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	60.40	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.027		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	1829.00		NIST Webbook
tb	645.81	K	Joback Method
tc	820.29	K	Joback Method
tf	323.20	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.82	J/mol×K	645.81	Joback Method
cpg	672.49	J/mol×K	674.89	Joback Method
cpg	689.35	J/mol×K	703.97	Joback Method
cpg	705.45	J/mol×K	733.05	Joback Method
cpg	720.80	J/mol×K	762.13	Joback Method
cpg	735.43	J/mol×K	791.21	Joback Method
cpg	749.36	J/mol×K	820.29	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=U373754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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