Dodecyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C17H32O2/c1-4-6-7-8-9-10-11-12-13-14-15-19-17(18)16(3)5-2/h5H,4,6-15H2,1

InchiKey: YSACBAGMGGQJJP-FZSIALSZSA-N

Formula: C17H32O2

SMILES: CC=C(C)C(=O)OCCCCCCCCCCCC

Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-69.99	kJ/mol	Joback Method
hf	-531.58	kJ/mol	Joback Method
hfus	41.47	kJ/mol	Joback Method
hvap	62.63	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.417		Crippen Method
mcvol	253.530	ml/mol	McGowan Method
pc	1325.20	kPa	Joback Method
rinpol	1930.00		NIST Webbook
tb	668.69	K	Joback Method
tc	842.79	K	Joback Method
tf	334.47	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.64	J/mol×K	668.69	Joback Method
cpg	728.72	J/mol×K	697.71	Joback Method
cpg	745.98	J/mol×K	726.72	Joback Method
cpg	762.44	J/mol×K	755.74	Joback Method
cpg	778.13	J/mol×K	784.75	Joback Method
cpg	793.08	J/mol×K	813.77	Joback Method
cpg	807.31	J/mol×K	842.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373750&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