Hexanoic acid, 3,5,5-trimethyl-, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C14H26O2/c1-11(2)7-8-16-13(15)9-12(3)10-14(4,5)6/h7,12H,8-10H2,1-6H3
InchiKey: HVBJKUSOHAZWLX-UHFFFAOYSA-N
Formula: C14H26O2
SMILES: CC(C)=CCOC(=O)CC(C)CC(C)(C)C
Mol. weight [g/mol]: 226.35

Physical Properties

Property code	Value	Unit	Source
gf	-94.85	kJ/mol	Joback Method
hf	-483.69	kJ/mol	Joback Method
hfus	22.76	kJ/mol	Joback Method
hvap	54.27	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.958		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	1441.00		NIST Webbook
rinpol	1441.00		NIST Webbook
tb	596.38	K	Joback Method
tc	784.89	K	Joback Method
tf	288.08	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.39	J/mol×K	596.38	Joback Method
cpg	568.26	J/mol×K	627.80	Joback Method
cpg	585.20	J/mol×K	659.22	Joback Method
cpg	601.26	J/mol×K	690.63	Joback Method
cpg	616.47	J/mol×K	722.05	Joback Method
cpg	630.86	J/mol×K	753.47	Joback Method
cpg	644.49	J/mol×K	784.89	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=U406928&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