Methyl valerenate

Inchi: InChI=1S/C16H24O2/c1-10-5-7-13(9-12(3)16(17)18-4)15-11(2)6-8-14(10)15/h9-10,13-14
InchiKey: OQZLCTPJWLOFKS-JLQUNKRQSA-N
Formula: C16H24O2
SMILES: COC(=O)C(C)=CC1CCC(C)C2CCC(C)=C12
Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	9.78	kJ/mol	Joback Method
hf	-369.32	kJ/mol	Joback Method
hfus	30.36	kJ/mol	Joback Method
hvap	62.05	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.878		Crippen Method
mcvol	213.420	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	1785.00		NIST Webbook
tb	676.55	K	Joback Method
tc	891.98	K	Joback Method
tf	370.08	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.88	J/mol×K	676.55	Joback Method
cpg	633.99	J/mol×K	712.45	Joback Method
cpg	652.88	J/mol×K	748.36	Joback Method
cpg	670.60	J/mol×K	784.26	Joback Method
cpg	687.20	J/mol×K	820.17	Joback Method
cpg	702.75	J/mol×K	856.07	Joback Method
cpg	717.29	J/mol×K	891.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R224965&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