«beta»-Cyclolavandulyl isovalerate

Inchi: InChI=1S/C15H26O2/c1-11(2)8-14(16)17-10-13-6-7-15(4,5)9-12(13)3/h11H,6-10H2,1-5H
InchiKey: DCWWZLVSQIFSJP-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: CC1=C(COC(=O)CC(C)C)CCC(C)(C)C1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-131.28	kJ/mol	Joback Method
hf	-498.61	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hvap	58.65	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.102		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
ripol	1815.00		NIST Webbook
tb	647.36	K	Joback Method
tc	852.79	K	Joback Method
tf	373.05	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.13	J/mol×K	647.36	Joback Method
cpg	609.34	J/mol×K	681.60	Joback Method
cpg	627.65	J/mol×K	715.84	Joback Method
cpg	645.14	J/mol×K	750.07	Joback Method
cpg	661.89	J/mol×K	784.31	Joback Method
cpg	678.01	J/mol×K	818.55	Joback Method
cpg	693.57	J/mol×K	852.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R418838&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume