Fragranyl 2-methylbutyrate

Inchi: InChI=1S/C15H26O2/c1-6-12(4)14(16)17-10-9-15(5)8-7-13(15)11(2)3/h12-13H,2,6-10H2
InchiKey: NRIGIDJZDUBPCH-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C=C(C)C1CCC1(C)CCOC(=O)C(C)CC
Mol. weight [g/mol]: 238.37
CAS: 51117-24-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.20	kJ/mol	Joback Method
hf	-425.83	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	55.79	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.958		Crippen Method
mcvol	214.490	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	1574.90		NIST Webbook
tb	621.59	K	Joback Method
tc	818.12	K	Joback Method
tf	334.33	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.12	J/mol×K	621.59	Joback Method
cpg	605.17	J/mol×K	654.34	Joback Method
cpg	623.28	J/mol×K	687.10	Joback Method
cpg	640.55	J/mol×K	719.85	Joback Method
cpg	657.08	J/mol×K	752.61	Joback Method
cpg	672.96	J/mol×K	785.36	Joback Method
cpg	688.30	J/mol×K	818.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51117249&Units=SI

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