3-(2-Methylbutyroxy)-nortropane

Inchi: InChI=1S/C12H21NO2/c1-3-8(2)12(14)15-11-6-9-4-5-10(7-11)13-9/h8-11,13H,3-7H2,1-2
InchiKey: UUNPOIBDFMMWPX-GGWWSXTCSA-N
Formula: C12H21NO2
SMILES: CCC(C)C(=O)OC1CC2CCC(C1)N2
Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
gf	-8.90	kJ/mol	Joback Method
hf	-390.34	kJ/mol	Joback Method
hfus	28.83	kJ/mol	Joback Method
hvap	57.69	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	1.859		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1532.00		NIST Webbook
tb	615.71	K	Joback Method
tc	830.47	K	Joback Method
tf	411.79	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.02	J/mol×K	615.71	Joback Method
cpg	511.55	J/mol×K	651.50	Joback Method
cpg	529.92	J/mol×K	687.30	Joback Method
cpg	547.18	J/mol×K	723.09	Joback Method
cpg	563.36	J/mol×K	758.88	Joback Method
cpg	578.51	J/mol×K	794.68	Joback Method
cpg	592.66	J/mol×K	830.47	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=R509503&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