Carbonic acid, monoamide, N-isobutyl-, octyl ester

Inchi: InChI=1S/C13H27NO2/c1-4-5-6-7-8-9-10-16-13(15)14-11-12(2)3/h12H,4-11H2,1-3H3,(H

InchiKey: SQBMGOCMBSQGBE-UHFFFAOYSA-N

Formula: C13H27NO2

SMILES: CCCCCCCCOC(=O)NCC(C)C

Mol. weight [g/mol]: 229.36

Physical Properties

Property code	Value	Unit	Source
gf	-88.39	kJ/mol	Joback Method
hf	-508.26	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	59.74	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.729		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	622.86	K	Joback Method
tc	797.16	K	Joback Method
tf	346.09	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.77	J/mol×K	622.86	Joback Method
cpg	590.24	J/mol×K	651.91	Joback Method
cpg	605.99	J/mol×K	680.96	Joback Method
cpg	621.03	J/mol×K	710.01	Joback Method
cpg	635.37	J/mol×K	739.06	Joback Method
cpg	649.02	J/mol×K	768.11	Joback Method
cpg	662.00	J/mol×K	797.16	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=U406437&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