Hexanamide, N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C13H27NO/c1-5-7-8-9-13(15)14(6-2)11-10-12(3)4/h12H,5-11H2,1-4H3
InchiKey: ZUWBTCIUTXQLDT-UHFFFAOYSA-N
Formula: C13H27NO
SMILES: CCCCCC(=O)N(CC)CCC(C)C
Mol. weight [g/mol]: 213.36

Physical Properties

Property code	Value	Unit	Source
gf	38.00	kJ/mol	Joback Method
hf	-361.98	kJ/mol	Joback Method
hfus	30.52	kJ/mol	Joback Method
hvap	52.93	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.461		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	562.71	K	Joback Method
tc	733.36	K	Joback Method
tf	303.67	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.86	J/mol×K	562.71	Joback Method
cpg	541.25	J/mol×K	591.15	Joback Method
cpg	557.86	J/mol×K	619.59	Joback Method
cpg	573.73	J/mol×K	648.04	Joback Method
cpg	588.87	J/mol×K	676.48	Joback Method
cpg	603.31	J/mol×K	704.92	Joback Method
cpg	617.08	J/mol×K	733.36	Joback Method

Sources

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=U415420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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