Propanamide, N-cyclohexyl-2-methyl

Inchi: InChI=1S/C10H19NO/c1-8(2)10(12)11-9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3,(H,11,12)
InchiKey: NPFIXJIFUHTLRP-UHFFFAOYSA-N
Formula: C10H19NO
SMILES: CC(C)C(=O)NC1CCCCC1
Mol. weight [g/mol]: 169.26
CAS: 6282-96-8

Physical Properties

Property code	Value	Unit	Source
gf	15.80	kJ/mol	Joback Method
hf	-259.80	kJ/mol	Joback Method
hfus	16.67	kJ/mol	Joback Method
hvap	51.08	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.091		Crippen Method
mcvol	152.450	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1392.00		NIST Webbook
rinpol	1392.00		NIST Webbook
tb	551.35	K	Joback Method
tc	763.83	K	Joback Method
tf	297.43	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.73	J/mol×K	551.35	Joback Method
cpg	401.25	J/mol×K	586.76	Joback Method
cpg	418.71	J/mol×K	622.18	Joback Method
cpg	435.13	J/mol×K	657.59	Joback Method
cpg	450.55	J/mol×K	693.01	Joback Method
cpg	464.99	J/mol×K	728.42	Joback Method
cpg	478.49	J/mol×K	763.83	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=C6282968&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