Propanenitrile, 3-(octylamino)-

Other names: 3-(octylamino)propiononitrile
Inchi: InChI=1S/C11H22N2/c1-2-3-4-5-6-7-10-13-11-8-9-12/h13H,2-8,10-11H2,1H3
InchiKey: AFXXFNVAHYRPIZ-UHFFFAOYSA-N
Formula: C11H22N2
SMILES: CCCCCCCCNCCC#N
Mol. weight [g/mol]: 182.31
CAS: 29504-89-0

Physical Properties

Property code	Value	Unit	Source
gf	264.31	kJ/mol	Joback Method
hf	-52.02	kJ/mol	Joback Method
hfus	30.85	kJ/mol	Joback Method
hvap	56.99	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	2.850		Crippen Method
mcvol	177.210	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
tb	603.33	K	Joback Method
tc	784.81	K	Joback Method
tf	331.38	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.75	J/mol×K	603.33	Joback Method
cpg	473.95	J/mol×K	633.58	Joback Method
cpg	487.50	J/mol×K	663.82	Joback Method
cpg	500.41	J/mol×K	694.07	Joback Method
cpg	512.72	J/mol×K	724.32	Joback Method
cpg	524.43	J/mol×K	754.56	Joback Method
cpg	535.58	J/mol×K	784.81	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=C29504890&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume