Propanenitrile, 3-(dodecylamino)-

Other names: 3-(dodecylamino)propiononitrile
Inchi: InChI=1S/C15H30N2/c1-2-3-4-5-6-7-8-9-10-11-14-17-15-12-13-16/h17H,2-12,14-15H2,1
InchiKey: DKRQDOPNZFOLQD-UHFFFAOYSA-N
Formula: C15H30N2
SMILES: CCCCCCCCCCCCNCCC#N
Mol. weight [g/mol]: 238.41
CAS: 4763-40-0

Physical Properties

Property code	Value	Unit	Source
gf	297.99	kJ/mol	Joback Method
hf	-134.58	kJ/mol	Joback Method
hfus	41.21	kJ/mol	Joback Method
hvap	65.90	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.411		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1402.74	kPa	Joback Method
tb	694.85	K	Joback Method
tc	872.72	K	Joback Method
tf	376.46	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.05	J/mol×K	694.85	Joback Method
cpg	688.35	J/mol×K	724.50	Joback Method
cpg	703.87	J/mol×K	754.14	Joback Method
cpg	718.65	J/mol×K	783.79	Joback Method
cpg	732.72	J/mol×K	813.43	Joback Method
cpg	746.10	J/mol×K	843.08	Joback Method
cpg	758.82	J/mol×K	872.72	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=C4763400&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume