

isopropyl-n-octyl-amine

Inchi:	InChI=1S/C11H25N/c1-4-5-6-7-8-9-10-12-11(2)3/h11-12H,4-10H2,1-3H3
InchiKey:	FXGYFSUEXFAPHG-UHFFFAOYSA-N
Formula:	C11H25N
SMILES:	CCCCCCCCNC(C)C
Mol. weight [g/mol]:	171.32
CAS:	25513-58-0

Physical Properties

Property code	Value	Unit	Source
gf	128.69	kJ/mol	Joback Method
hf	-222.18	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.345		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1189.00		NIST Webbook
rinpol	1189.00		NIST Webbook
tb	500.81	K	Joback Method
tc	669.39	K	Joback Method
tf	251.39	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.58	J/molxK	500.81	Joback Method
cpg	432.13	J/molxK	528.91	Joback Method
cpg	448.02	J/molxK	557.00	Joback Method
cpg	463.26	J/molxK	585.10	Joback Method
cpg	477.87	J/molxK	613.19	Joback Method
cpg	491.87	J/molxK	641.29	Joback Method
cpg	505.27	J/molxK	669.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25513580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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