

methylheptyl-amine

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C8H19N/c1-3-4-5-6-7-8-9-2/h9H,3-8H2,1-2H3

LTGYRKOQQQWWAF-UHFFFAOYSA-N

C8H19N

CCCCCCCNC

129.24

Physical Properties

Property code	Value	Unit	Source
gf	105.87	kJ/mol	Joback Method
hf	-154.98	kJ/mol	Joback Method
hfus	21.57	kJ/mol	Joback Method
hvap	39.84	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.176		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	985.00		NIST Webbook
rinpol	985.00		NIST Webbook
tb	432.61	K	Joback Method
tc	600.98	K	Joback Method
tf	232.58	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.38	J/mol×K	432.61	Joback Method
cpg	293.01	J/mol×K	460.67	Joback Method
cpg	306.12	J/mol×K	488.73	Joback Method
cpg	318.72	J/mol×K	516.80	Joback Method
cpg	330.83	J/mol×K	544.86	Joback Method
cpg	342.46	J/mol×K	572.92	Joback Method
cpg	353.63	J/mol×K	600.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R521578&Units=SI
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

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

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