

Methyldiallylamine

Other names:	2-Propen-1-amine, N-methyl-N-2-propenyl-Diallylmethylamine N,N-Di(2-propenyl)-N-methylamine N-methyldiallylamine
Inchi:	InChI=1S/C7H13N/c1-4-6-8(3)7-5-2/h4-5H,1-2,6-7H2,3H3
InchiKey:	WGESLFUSXZBFQF-UHFFFAOYSA-N
Formula:	C7H13N
SMILES:	C=CCN(C)CC=C
Mol. weight [g/mol]:	111.18
CAS:	2424-01-3

Physical Properties

Property code	Value	Unit	Source
gf	294.52	kJ/mol	Joback Method
hf	130.58	kJ/mol	Joback Method
hfus	14.35	kJ/mol	Joback Method
hvap	31.88	kJ/mol	Joback Method
ie	8.40 ± 0.30	eV	NIST Webbook
log10ws	-1.03		Crippen Method
logp	1.290		Crippen Method
mcvol	110.870	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	385.00	K	NIST Webbook
tc	534.65	K	Joback Method
tf	197.60	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.10	J/mol×K	365.36	Joback Method
cpg	205.06	J/mol×K	393.58	Joback Method
cpg	216.48	J/mol×K	421.79	Joback Method
cpg	227.36	J/mol×K	450.01	Joback Method

cpg	237.73	J/mol×K	478.22	Joback Method
cpg	247.61	J/mol×K	506.44	Joback Method
cpg	257.02	J/mol×K	534.65	Joback Method

Sources

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=C2424013&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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

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