1-Butanaine, 3-methyl, N-(2-propenyl)

Inchi: InChI=1S/C8H17N/c1-4-6-9-7-5-8(2)3/h4,8-9H,1,5-7H2,2-3H3
InchiKey: ATPUSBMSUZPBCH-UHFFFAOYSA-N
Formula: C8H17N
SMILES: C=CCNCCC(C)C
Mol. weight [g/mol]: 127.23

Physical Properties

Property code	Value	Unit	Source
gf	191.27	kJ/mol	Joback Method
hf	-34.83	kJ/mol	Joback Method
hfus	16.77	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.808		Crippen Method
mcvol	129.260	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
tb	428.85	K	Joback Method
tc	604.40	K	Joback Method
tf	215.82	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.32	J/mol×K	428.85	Joback Method
cpg	276.80	J/mol×K	458.11	Joback Method
cpg	289.70	J/mol×K	487.37	Joback Method
cpg	302.05	J/mol×K	516.62	Joback Method
cpg	313.87	J/mol×K	545.88	Joback Method
cpg	325.16	J/mol×K	575.14	Joback Method
cpg	335.95	J/mol×K	604.40	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=R19630&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume