

1-Bromo-3,5,5-trimethylhexane

Inchi:	InChI=1S/C9H19Br/c1-8(5-6-10)7-9(2,3)4/h8H,5-7H2,1-4H3
InchiKey:	JUHBYLSCAJAHEH-UHFFFAOYSA-N
Formula:	C9H19Br
SMILES:	CC(CCBBr)CC(C)(C)C
Mol. weight [g/mol]:	207.15
CAS:	50915-80-5

Physical Properties

Property code	Value	Unit	Source
gf	39.62	kJ/mol	Joback Method
hf	-216.79	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	40.38	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.844		Crippen Method
mcvol	155.170	ml/mol	McGowan Method
pc	2535.37	kPa	Joback Method
tb	467.81	K	Joback Method
tc	662.70	K	Joback Method
tf	238.41	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.77	J/molxK	467.81	Joback Method
cpg	338.39	J/molxK	500.29	Joback Method
cpg	353.15	J/molxK	532.77	Joback Method
cpg	367.08	J/molxK	565.25	Joback Method
cpg	380.23	J/molxK	597.74	Joback Method
cpg	392.64	J/molxK	630.22	Joback Method
cpg	404.35	J/molxK	662.70	Joback Method
dvisc	0.0094024	Paxs	238.41	Joback Method
dvisc	0.0034670	Paxs	276.64	Joback Method

dvisc	0.0016289	Paxs	314.88	Joback Method
dvisc	0.0009013	Paxs	353.11	Joback Method
dvisc	0.0005599	Paxs	391.34	Joback Method
dvisc	0.0003785	Paxs	429.58	Joback Method
dvisc	0.0002728	Paxs	467.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50915805&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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