

Geranyl bromide

Other names:	2,6-Octadiene, 1-bromo-3,7-dimethyl-, (E)- (2E)-1-Bromo-3,7-dimethyl-2,6-octadiene trans-Geranyl bromide 2,6-Octadiene, 1-bromo-3,7-dimethyl-, (2E)- (E)-1-bromo-3,7-dimethylocta-2,6-diene
Inchi:	InChI=1S/C10H17Br/c1-9(2)5-4-6-10(3)7-8-11/h5,7H,4,6,8H2,1-3H3/b10-7+
InchiKey:	JSCUZAYKVZXXQE-JXMROGBWSA-N
Formula:	C10H17Br
SMILES:	CC(C)=CCCC(C)=CCBr
Mol. weight [g/mol]:	217.15
CAS:	6138-90-5

Physical Properties

Property code	Value	Unit	Source
gf	190.98	kJ/mol	Joback Method
hf	-8.54	kJ/mol	Joback Method
hfus	24.73	kJ/mol	Joback Method
hvap	44.37	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.074		Crippen Method
mcvol	160.660	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1282.00		NIST Webbook
tb	502.44	K	Joback Method
tc	703.93	K	Joback Method
tf	224.18	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.35	J/molxK	502.44	Joback Method
cpg	344.90	J/molxK	536.02	Joback Method
cpg	358.59	J/molxK	569.60	Joback Method

cpg	371.49	J/mol×K	603.18	Joback Method
cpg	383.64	J/mol×K	636.77	Joback Method
cpg	395.11	J/mol×K	670.35	Joback Method
cpg	405.94	J/mol×K	703.93	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.70	K	1.60	NIST Webbook

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=C6138905&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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