

5-Bromo-2-methyl-2-pentene

Inchi:	InChI=1S/C6H11Br/c1-6(2)4-3-5-7/h4H,3,5H2,1-2H3
InchiKey:	UNXURIHDFUQNOC-UHFFFAOYSA-N
Formula:	C6H11Br
SMILES:	CC(C)=CCBr
Mol. weight [g/mol]:	163.06
CAS:	2270-59-9

Physical Properties

Property code	Value	Unit	Source
gf	85.63	kJ/mol	Joback Method
hf	-33.41	kJ/mol	Joback Method
hfus	15.47	kJ/mol	Joback Method
hvap	35.42	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.738		Crippen Method
mcvol	108.600	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	406.88	K	Joback Method
tc	604.16	K	Joback Method
tf	198.14	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.37	J/molxK	406.88	Joback Method
cpg	192.88	J/molxK	439.76	Joback Method
cpg	202.80	J/molxK	472.64	Joback Method
cpg	212.17	J/molxK	505.52	Joback Method
cpg	221.01	J/molxK	538.40	Joback Method
cpg	229.36	J/molxK	571.28	Joback Method
cpg	237.25	J/molxK	604.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50173e+01
Coeff. B	-3.81204e+03
Coeff. C	-5.96200e+01
Temperature range (K), min.	318.42
Temperature range (K), max.	452.38

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2270599&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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