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)=CCCBr
Mol. weight [g/mol]: 163.06
CAS: 2270-59-9

Physical Properties

Property code	Value	Unit	Source
af	0.3645		Cheméo Relay (1.0)
gf	85.63	kJ/mol	Joback Method
hf	-59.71	kJ/mol	Cheméo Relay (1.0)
hfus	15.47	kJ/mol	Joback Method
hvap	44.81	kJ/mol	Cheméo Relay (1.0)
ie	8.84	eV	Cheméo Relay (1.0)
log10ws	-3.01		Cheméo Relay (1.0)
logp	2.738		Crippen Method
mcvol	108.600	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	604.25	K	Cheméo Relay (1.0)
tf	205.39	K	Cheméo Relay (1.0)
vc	0.384	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2270599&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

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