3-BROMO-2,2-DIMETHYL-1-PROPANOL

Inchi: InChI=1S/C5H11BrO/c1-5(2,3-6)4-7/h7H,3-4H2,1-2H3
InchiKey: KQOQXYPZBYTICM-UHFFFAOYSA-N
Formula: C5H11BrO
SMILES: CC(C)(CO)CBr
Mol. weight [g/mol]: 167.05

Physical Properties

Property code	Value	Unit	Source
af	0.6071		Cheméo Relay (1.0)
gf	-128.44	kJ/mol	Joback Method
hf	-312.73	kJ/mol	Cheméo Relay (1.0)
hfus	10.66	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Cheméo Relay (1.0)
ie	9.97	eV	Cheméo Relay (1.0)
log10ws	-1.20		Cheméo Relay (1.0)
logp	1.400		Crippen Method
mcvol	104.680	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	458.70	K	NIST Webbook
tc	678.40	K	Cheméo Relay (1.0)
tf	298.54	K	Cheméo Relay (1.0)
vc	0.364	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.92	J/mol×K	468.91	Joback Method
cpg	215.94	J/mol×K	500.39	Joback Method
cpg	224.42	J/mol×K	531.87	Joback Method
cpg	232.39	J/mol×K	563.35	Joback Method
cpg	239.87	J/mol×K	594.83	Joback Method
cpg	246.89	J/mol×K	626.30	Joback Method
cpg	253.50	J/mol×K	657.78	Joback Method
dvisc	0.0312926	Pa×s	269.15	Joback Method

dvisc	0.0090766	Pa×s	302.44	Joback Method
dvisc	0.0033652	Pa×s	335.74	Joback Method
dvisc	0.0014923	Pa×s	369.03	Joback Method
dvisc	0.0007571	Pa×s	402.32	Joback Method
dvisc	0.0004261	Pa×s	435.62	Joback Method
dvisc	0.0002602	Pa×s	468.91	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40894006&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
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
ie: Ionization energy
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