PROPIONYL BROMIDE

Other names: Propanoyl-bromide-
Inchi: InChI=1S/C3H5BrO/c1-2-3(4)5/h2H2,1H3
InchiKey: RIBFXMJCUYXJDZ-UHFFFAOYSA-N
Formula: C3H5BrO
SMILES: CCC(=O)Br
Mol. weight [g/mol]: 136.98

Physical Properties

Property code	Value	Unit	Source
af	0.3620		Cheméo Relay (1.0)
gf	-140.22	kJ/mol	Joback Method
hf	-197.74	kJ/mol	Cheméo Relay (1.0)
hfus	10.41	kJ/mol	Joback Method
hvap	29.71	kJ/mol	Cheméo Relay (1.0)
ie	10.18	eV	Cheméo Relay (1.0)
log10ws	-0.86		Cheméo Relay (1.0)
logp	1.318		Crippen Method
mcvol	72.200	ml/mol	McGowan Method
pc	5296.96	kPa	Joback Method
tb	376.70	K	NIST Webbook
tb	372.00 ± 4.00	K	NIST Webbook
tc	565.47	K	Cheméo Relay (1.0)
tf	194.14	K	Cheméo Relay (1.0)
vc	0.268	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	105.72	J/mol×K	388.07	Joback Method
cpg	111.35	J/mol×K	421.65	Joback Method
cpg	116.70	J/mol×K	455.23	Joback Method
cpg	121.76	J/mol×K	488.81	Joback Method
cpg	126.56	J/mol×K	522.39	Joback Method
cpg	131.10	J/mol×K	555.97	Joback Method

cpg	135.39	J/mol×K	589.55	Joback Method
dvisc	0.0031172	Pa×s	233.30	Joback Method
dvisc	0.0019296	Pa×s	259.10	Joback Method
dvisc	0.0013029	Pa×s	284.89	Joback Method
dvisc	0.0009390	Pa×s	310.69	Joback Method
dvisc	0.0007116	Pa×s	336.48	Joback Method
dvisc	0.0005609	Pa×s	362.27	Joback Method
dvisc	0.0004564	Pa×s	388.07	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C598221&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