2H-Pyran, 2-(bromomethyl)tetrahydro-

Other names: 2-(Bromomethyl)tetrahydro-2H-pyran
Pyran, 2-(bromomethyl)tetrahydro-
Inchi: InChI=1S/C6H11BrO/c7-5-6-3-1-2-4-8-6/h6H,1-5H2
InchiKey: MHNWCBOXPOLLIB-UHFFFAOYSA-N
Formula: C6H11BrO
SMILES: BrCC1CCCCO1
Mol. weight [g/mol]: 179.06
CAS: 34723-82-5

Physical Properties

Property code	Value	Unit	Source
gf	-47.71	kJ/mol	Joback Method
hf	-218.52	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	40.32	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.950		Crippen Method
mcvol	107.910	ml/mol	McGowan Method
pc	4277.45	kPa	Joback Method
tb	426.20	K	NIST Webbook
tc	674.65	K	Joback Method
tf	251.13	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.43	J/mol×K	449.34	Joback Method
cpg	268.70	J/mol×K	637.10	Joback Method
cpg	257.63	J/mol×K	599.55	Joback Method
cpg	245.80	J/mol×K	562.00	Joback Method
cpg	233.17	J/mol×K	524.44	Joback Method
cpg	219.73	J/mol×K	486.89	Joback Method
cpg	279.04	J/mol×K	674.65	Joback Method

dvisc	0.0004172	Pa×s	449.34	Joback Method
dvisc	0.0005449	Pa×s	416.31	Joback Method
dvisc	0.0007450	Pa×s	383.27	Joback Method
dvisc	0.0010807	Pa×s	350.24	Joback Method
dvisc	0.0016939	Pa×s	317.20	Joback Method
dvisc	0.0029474	Pa×s	284.17	Joback Method
dvisc	0.0059330	Pa×s	251.13	Joback Method

Sources

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=C34723825&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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

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