Cycloheptane, bromo-

Other names:	Bromocycloheptane
	Cycloheptyl bromide
Inchi:	InChI=1S/C7H13Br/c8-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey:	LOXORFRCPXUORP-UHFFFAOYSA-N
Formula:	C7H13Br
SMILES:	BrC1CCCCCC1
Mol. weight [g/mol]:	177.08
CAS:	2404-35-5

Physical Properties

Property code	Value	Unit	Source
gf	34.73	kJ/mol	Joback Method
hf	-113.32	kJ/mol	Joback Method
hfus	8.91	kJ/mol	Joback Method
hvap	38.21	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.104		Crippen Method
mcvol	116.130	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
rinpol	1157.00		NIST Webbook
rinpol	1157.00		NIST Webbook
tb	449.54	K	Joback Method
tc	681.95	K	Joback Method
tf	232.31	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.63	J/mol×K	449.54	Joback Method
cpg	233.75	J/mol×K	488.28	Joback Method
cpg	249.85	J/mol×K	527.01	Joback Method
cpg	264.98	J/mol×K	565.75	Joback Method
cpg	279.16	J/mol×K	604.48	Joback Method

cpg	292.41	J/mol×K	643.22	Joback Method
cpg	304.77	J/mol×K	681.95	Joback Method
dvisc	0.0086730	Pa×s	232.31	Joback Method
dvisc	0.0034426	Pa×s	268.51	Joback Method
dvisc	0.0017020	Pa×s	304.72	Joback Method
dvisc	0.0009772	Pa×s	340.92	Joback Method
dvisc	0.0006242	Pa×s	377.13	Joback Method
dvisc	0.0004313	Pa×s	413.33	Joback Method
dvisc	0.0003162	Pa×s	449.54	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	1.30	NIST Webbook
tbrp	356.00	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2404355&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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