

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:	BrC1CCCCC1
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
mvol	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	m ³ /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/molxK	643.22	Joback Method
cpg	304.77	J/molxK	681.95	Joback Method
dvisc	0.0086730	Paxs	232.31	Joback Method
dvisc	0.0034426	Paxs	268.51	Joback Method
dvisc	0.0017020	Paxs	304.72	Joback Method
dvisc	0.0009772	Paxs	340.92	Joback Method
dvisc	0.0006242	Paxs	377.13	Joback Method
dvisc	0.0004313	Paxs	413.33	Joback Method
dvisc	0.0003162	Paxs	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2404355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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