

Bromociclen

Other names:	Bicyclo[2.2.1]hept-2-ene, 5-(bromomethyl)-1,2,3,4,7,7-hexachloro-2-Norbornene, 5-(bromomethyl)-1,2,3,4,7,7-hexachloro-Alugan Bromodan ENT 23393 SD 2774 Bromocyclen Bromocyclene Bromomethylhexachlorobicycloheptene 5-(Bromomethyl)-1,2,3,4,7,7-hexachlorobicyclo(2.2.1)hept-2-ene 5-(Bromomethyl)-1,2,3,4,7,7-hexachloro-2-norbornene 5-(Bromomethyl)-1,2,3,4,7,7-hexachloro-norbornene Bromomethyl-1,2,3,4,7,7-hexachloro-2-norbornene
Inchi:	InChI=1S/C8H5BrCl6/c9-2-3-1-6(12)4(10)5(11)7(3,13)8(6,14)15/h3H,1-2H2
InchiKey:	DAASOABUJRMZAD-UHFFFAOYSA-N
Formula:	C8H5BrCl6
SMILES:	<chem>C1C=C(Cl)C2(Cl)C(CBr)CC1(Cl)C2(Cl)Cl</chem>
Mol. weight [g/mol]:	393.75
CAS:	1715-40-8

Physical Properties

Property code	Value	Unit	Source
gf	47.43	kJ/mol	Joback Method
hf	-97.24	kJ/mol	Joback Method
hfus	24.80	kJ/mol	Joback Method
hvap	63.69	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.233		Crippen Method
mcvol	188.500	ml/mol	McGowan Method
pc	3159.72	kPa	Joback Method
tb	691.43	K	Joback Method
tc	971.25	K	Joback Method
tf	540.62	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.49	J/mol×K	691.43	Joback Method
cpg	370.66	J/mol×K	738.07	Joback Method
cpg	379.57	J/mol×K	784.70	Joback Method
cpg	389.90	J/mol×K	831.34	Joback Method
cpg	402.35	J/mol×K	877.98	Joback Method
cpg	417.60	J/mol×K	924.62	Joback Method
cpg	436.34	J/mol×K	971.25	Joback Method

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=C1715408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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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