2,12-Dibromocyclododecanone

Other names: Cyclododecanone, 2,12-dibromo-
Inchi: InChI=1S/C12H20Br2O/c13-10-8-6-4-2-1-3-5-7-9-11(14)12(10)15/h10-11H,1-9H2
InchiKey: CLAFKWVRFMBEBC-UHFFFAOYSA-N
Formula: C12H20Br2O
SMILES: O=C1C(Br)CCCCCCCCCC1Br
Mol. weight [g/mol]: 340.10
CAS: 24459-40-3

Physical Properties

Property code	Value	Unit	Source
gf	-99.65	kJ/mol	Joback Method
hf	-379.03	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.607		Crippen Method
mcvol	205.650	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	714.60	K	Joback Method
tc	994.19	K	Joback Method
tf	394.84	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.23	J/mol×K	714.60	Joback Method
cpg	575.64	J/mol×K	761.20	Joback Method
cpg	596.76	J/mol×K	807.80	Joback Method
cpg	615.50	J/mol×K	854.40	Joback Method
cpg	631.82	J/mol×K	900.99	Joback Method
cpg	645.63	J/mol×K	947.59	Joback Method
cpg	656.88	J/mol×K	994.19	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=C24459403&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
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