5,9-Cyclododecadien-1,2-diol

Inchi: InChI=1S/C12H20O2/c13-11-9-7-5-3-1-2-4-6-8-10-12(11)14/h3-6,11-14H,1-2,7-10H2/b5-
InchiKey: BHYILZSOXKSYCF-GGWOSOGESA-N
Formula: C12H20O2
SMILES: OC1CCC=CCCC=CCCC1O
Mol. weight [g/mol]: 196.29
CAS: 15786-26-2

Physical Properties

Property code	Value	Unit	Source
gf	-219.42	kJ/mol	Joback Method
hf	-482.89	kJ/mol	Joback Method
hfus	17.76	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.175		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	697.14	K	Joback Method
tc	905.76	K	Joback Method
tf	330.18	K	Joback Method
vc	0.602	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.91	J/mol×K	697.14	Joback Method
cpg	581.15	J/mol×K	870.99	Joback Method
cpg	568.94	J/mol×K	836.22	Joback Method
cpg	555.50	J/mol×K	801.45	Joback Method
cpg	540.84	J/mol×K	766.68	Joback Method
cpg	524.97	J/mol×K	731.91	Joback Method
cpg	592.12	J/mol×K	905.76	Joback Method
dvisc	0.0000029	Pa×s	697.14	Joback Method
dvisc	0.0000065	Pa×s	635.98	Joback Method

dvisc	0.0000173	Pa×s	574.82	Joback Method
dvisc	0.0000582	Pa×s	513.66	Joback Method
dvisc	0.0002709	Pa×s	452.50	Joback Method
dvisc	0.0020396	Pa×s	391.34	Joback Method
dvisc	0.0324360	Pa×s	330.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15786262&Units=SI

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

Latest version available from:

https://www.chemeo.com/cid/85-168-2/5-9-Cyclododecadien-1-2-diol.pdf

Generated by Cheméo on 2024-10-12 07:40:35.147030419 +0000 UTC m=+3299697.783999668.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.