Chalcogran, isomer # 1

Inchi: InChI=1S/C9H16O2/c1-2-8-4-6-9(11-8)5-3-7-10-9/h8H,2-7H2,1H3
InchiKey: DCWKALWZHORJAO-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCC1CCC2(CCCO2)O1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-67.63	kJ/mol	Joback Method
hf	-350.73	kJ/mol	Joback Method
hfus	18.70	kJ/mol	Joback Method
hvap	43.84	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.082		Crippen Method
mcvol	127.690	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
ripol	1343.00		NIST Webbook
ripol	1343.00		NIST Webbook
tb	485.75	K	Joback Method
tc	709.46	K	Joback Method
tf	293.55	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.72	J/mol×K	485.75	Joback Method
cpg	326.56	J/mol×K	523.04	Joback Method
cpg	343.99	J/mol×K	560.32	Joback Method
cpg	360.14	J/mol×K	597.61	Joback Method
cpg	375.18	J/mol×K	634.89	Joback Method
cpg	389.26	J/mol×K	672.18	Joback Method
cpg	402.52	J/mol×K	709.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R607835&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume