trans-Diallate

Inchi: InChI=1S/C10H17Cl2NOS/c1-7(2)13(8(3)4)10(14)15-6-9(12)5-11/h5,7-8H,6H2,1-4H3/b9
InchiKey: SPANOECCGNXGNR-UITAMQMPSA-N
Formula: C10H17Cl2NOS
SMILES: CC(C)N(C(=O)SCC(Cl)=CCl)C(C)C
Mol. weight [g/mol]: 270.22
CAS: 17708-58-6

Physical Properties

Property code	Value	Unit	Source
gf	91.23	kJ/mol	Joback Method
hf	-187.52	kJ/mol	Joback Method
hfus	30.65	kJ/mol	Joback Method
hvap	61.49	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.277		Crippen Method
mcvol	199.840	ml/mol	McGowan Method
pc	2265.42	kPa	Joback Method
ripol	2266.00		NIST Webbook
tb	641.31	K	Joback Method
tc	857.18	K	Joback Method
tf	330.06	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.54	J/mol×K	641.31	Joback Method
cpg	486.39	J/mol×K	677.29	Joback Method
cpg	499.32	J/mol×K	713.27	Joback Method
cpg	511.40	J/mol×K	749.25	Joback Method
cpg	522.66	J/mol×K	785.22	Joback Method
cpg	533.15	J/mol×K	821.20	Joback Method
cpg	542.93	J/mol×K	857.18	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=C17708586&Units=SI

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