

Diethyl dithiol oxalate

Inchi:	InChI=1S/C6H10O2S2/c1-3-9-5(7)6(8)10-4-2/h3-4H2,1-2H3
InchiKey:	AOPOCMMRDUZGAS-UHFFFAOYSA-N
Formula:	C6H10O2S2
SMILES:	CCSC(=O)C(=O)SCC
Mol. weight [g/mol]:	178.27
CAS:	615-85-0

Physical Properties

Property code	Value	Unit	Source
gf	-191.96	kJ/mol	Joback Method
hf	-308.59	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	56.08	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.546		Crippen Method
mcvol	131.240	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	581.98	K	Joback Method
tc	812.25	K	Joback Method
tf	326.04	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.02	J/molxK	581.98	Joback Method
cpg	291.40	J/molxK	620.36	Joback Method
cpg	301.15	J/molxK	658.74	Joback Method
cpg	310.29	J/molxK	697.11	Joback Method
cpg	318.80	J/molxK	735.49	Joback Method
cpg	326.68	J/molxK	773.87	Joback Method
cpg	333.92	J/molxK	812.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615850&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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