

Ethyl 1,3-dithiolane-2-carboxylate

Other names:	2-Carboethoxydithiolane 2-Carboethoxy-1,3-dithiolane 1,3-Dithiolane-2-carboxylic acid, ethyl ester
Inchi:	InChI=1S/C6H10O2S2/c1-2-8-5(7)6-9-3-4-10-6/h6H,2-4H2,1H3
InchiKey:	OMCSHTHLIQOHDD-UHFFFAOYSA-N
Formula:	C6H10O2S2
SMILES:	CCOC(=O)C1SCCS1
Mol. weight [g/mol]:	178.27
CAS:	20461-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-118.01	kJ/mol	Joback Method
hf	-260.97	kJ/mol	Joback Method
hfus	15.33	kJ/mol	Joback Method
hvap	49.99	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.356		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	523.91	K	Joback Method
tc	761.34	K	Joback Method
tf	407.34	K	Joback Method
vc	0.428	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.39	J/molxK	523.91	Joback Method
cpg	278.19	J/molxK	563.48	Joback Method
cpg	290.21	J/molxK	603.05	Joback Method
cpg	301.48	J/molxK	642.63	Joback Method
cpg	312.01	J/molxK	682.20	Joback Method
cpg	321.83	J/molxK	721.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20461998&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

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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