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]: 178.28

Physical Properties

Property code	Value	Unit	Source
hf	-377.63	kJ/mol	Cheméo Relay (1.0)
hfus	15.33	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Cheméo Relay (1.0)
ie	8.68	eV	Cheméo Relay (1.0)
log10ws	-1.52		Cheméo Relay (1.0)
logp	1.356		Crippen Method
mcvol	124.680	ml/mol	McGowan Method
pc	4005.77	kPa	Joback Method
tb	521.15	K	Cheméo Relay (1.0)
tc	743.91	K	Cheméo Relay (1.0)
tf	321.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.39	J/mol×K	523.91	Joback Method
cpg	278.19	J/mol×K	563.48	Joback Method
cpg	290.21	J/mol×K	603.05	Joback Method
cpg	301.48	J/mol×K	642.63	Joback Method
cpg	312.01	J/mol×K	682.20	Joback Method
cpg	321.83	J/mol×K	721.77	Joback Method
cpg	330.95	J/mol×K	761.34	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20461998&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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