Ethyl 1,3-dithiane-2-carboxylate

Other names:	Carboethoxy-1,3-dithiane
	2-Carboethoxy-1,3-dithiane
	1,3-Dithiane-2-carboxylic acid ethyl ester
Inchi:	InChI=1S/C7H12O2S2/c1-2-9-6(8)7-10-4-3-5-11-7/h7H,2-5H2,1H3
InchiKey:	ANEDZEVDORCLPM-UHFFFAOYSA-N
Formula:	C7H12O2S2
SMILES:	CCOC(=O)C1SCCCS1
Mol. weight [g/mol]:	192.30
CAS:	20462-00-4

Physical Properties

Property code	Value	Unit	Source
gf	-121.69	kJ/mol	Joback Method
hf	-287.77	kJ/mol	Joback Method
hfus	15.82	kJ/mol	Joback Method
hvap	52.39	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.746		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
pc	3668.65	kPa	Joback Method
tb	551.06	K	Joback Method
tc	792.65	K	Joback Method
tf	415.09	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.85	J/mol×K	551.06	Joback Method
cpg	324.68	J/mol×K	591.32	Joback Method
cpg	338.59	J/mol×K	631.59	Joback Method
cpg	351.60	J/mol×K	671.85	Joback Method
cpg	363.72	J/mol×K	712.12	Joback Method
cpg	374.97	J/mol×K	752.38	Joback Method

cpg	385.36	J/mol×K	792.65	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	0.03	NIST Webbook

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=C20462004&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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