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]: 192.31

Physical Properties

Property code	Value	Unit	Source
hfus	15.82	kJ/mol	Joback Method
logp	1.746		Crippen Method
mcvol	138.770	ml/mol	McGowan Method
tb	541.45	K	Cheméo Relay (1.0)

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

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=C20462004&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure