Isoprothiolane

Other names:	Di-isopropyl 1,3-dithiolane-2-ylidenemalonate
	Fudiolan
	Fuji 1
	Fujione
	IPT
	Isoprothiolane
	NKK 100
	NNF-109
	SS 11946
	IPT (pesticide)
	Bis(1-methylethyl) 1,3-dithiolan-2-ylidenepropanedioate
	Diisopropyl 2-(1,3-dithiolan-2-ylidene)propanedioate
	Malonic acid, 2-(1,3-dithiolan-2-ylidene), diisopropyl ester
	Propanedioic acid, 2-(1,3-dithiolan-2-ylidene)-, 1,3-bis(1-methylethyl) ester
Inchi:	InChI=1S/C12H18O4S2/c1-7(2)15-10(13)9(11(14)16-8(3)4)12-17-5-6-18-12/h7-8H,5-6H2
InchiKey:	UFHLMYOGRXOCSL-UHFFFAOYSA-N
Formula:	C12H18O4S2
SMILES:	CC(C)OC(=O)C(C(=O)OC(C)C)=C1SCCS1
Mol. weight [g/mol]:	290.41

Physical Properties

Property code	Value	Unit	Source
hfus	24.55	kJ/mol	Joback Method
logp	2.581		Crippen Method
mcvol	212.360	ml/mol	McGowan Method
rinpol	2175.00		NIST Webbook
rinpol	2194.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2167.00		NIST Webbook
rinpol	2194.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2167.00		NIST Webbook
ripol	3254.00		NIST Webbook
tb	582.42	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.55	J/mol×K	747.79	Joback Method
cpg	588.07	J/mol×K	786.70	Joback Method
cpg	601.53	J/mol×K	825.60	Joback Method
cpg	613.95	J/mol×K	864.51	Joback Method
cpg	625.36	J/mol×K	903.41	Joback Method
cpg	635.81	J/mol×K	942.32	Joback Method
cpg	645.32	J/mol×K	981.23	Joback Method

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=C50512351&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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