Diethyl fluoromalonate

Other names:	Ethyl fluoromalonate
	Propanedioic acid, fluoro-, diethyl ester
	Malonic acid, fluoro-, diethyl ester
	Fluoromalonic acid diethyl ester
	Monofluoromalonic acid diethyl ester
Inchi:	InChI=1S/C7H11FO4/c1-3-11-6(9)5(8)7(10)12-4-2/h5H,3-4H2,1-2H3
InchiKey:	GOWQBFVDZPZZFA-UHFFFAOYSA-N
Formula:	C7H11FO4
SMILES:	CCOC(=O)C(F)C(=O)OCC
Mol. weight [g/mol]:	178.16
CAS:	685-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-657.03	kJ/mol	Joback Method
hf	-878.80	kJ/mol	Joback Method
hfus	19.02	kJ/mol	Joback Method
hvap	48.28	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.451		Crippen Method
mcvol	126.140	ml/mol	McGowan Method
pc	2969.80	kPa	Joback Method
tb	510.97	K	Joback Method
tc	691.68	K	Joback Method
tf	298.56	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.92	J/mol×K	510.97	Joback Method
cpg	297.13	J/mol×K	541.09	Joback Method
cpg	306.97	J/mol×K	571.21	Joback Method
cpg	316.45	J/mol×K	601.32	Joback Method

cpg	325.55	J/mol×K	631.44	Joback Method
cpg	334.26	J/mol×K	661.56	Joback Method
cpg	342.58	J/mol×K	691.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.50 ± 0.50	K	2.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C685881&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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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