Diethylmalonic acid, ethyl 2-fluoroethyl ester

Inchi: InChI=1S/C11H19FO4/c1-4-11(5-2,9(13)15-6-3)10(14)16-8-7-12/h4-8H2,1-3H3
InchiKey: OFSKSHDIOCVPMK-UHFFFAOYSA-N
Formula: C11H19FO4
SMILES: CCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 234.26

Physical Properties

Property code	Value	Unit	Source
gf	-618.07	kJ/mol	Joback Method
hf	-964.83	kJ/mol	Joback Method
hfus	25.49	kJ/mol	Joback Method
hvap	56.28	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	1.869		Crippen Method
mcvol	182.500	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
rinpol	1292.00		NIST Webbook
rinpol	1292.00		NIST Webbook
tb	599.70	K	Joback Method
tc	779.69	K	Joback Method
tf	361.06	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.31	J/mol×K	599.70	Joback Method
cpg	490.23	J/mol×K	629.70	Joback Method
cpg	503.48	J/mol×K	659.70	Joback Method
cpg	516.07	J/mol×K	689.70	Joback Method
cpg	528.02	J/mol×K	719.69	Joback Method
cpg	539.32	J/mol×K	749.69	Joback Method
cpg	550.01	J/mol×K	779.69	Joback Method

Sources

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=U370857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume