Diethylmalonic acid, butyl 2-fluoroethyl ester

Inchi: InChI=1S/C13H23FO4/c1-4-7-9-17-11(15)13(5-2,6-3)12(16)18-10-8-14/h4-10H2,1-3H3
InchiKey: QZFYKLIPMOHSBU-UHFFFAOYSA-N
Formula: C13H23FO4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 262.32

Physical Properties

Property code	Value	Unit	Source
gf	-601.23	kJ/mol	Joback Method
hf	-1006.11	kJ/mol	Joback Method
hfus	30.67	kJ/mol	Joback Method
hvap	60.73	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.649		Crippen Method
mcvol	210.680	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	1464.00		NIST Webbook
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tb	645.46	K	Joback Method
tc	823.05	K	Joback Method
tf	383.60	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.17	J/mol×K	645.46	Joback Method
cpg	594.19	J/mol×K	675.06	Joback Method
cpg	608.48	J/mol×K	704.66	Joback Method
cpg	622.04	J/mol×K	734.26	Joback Method
cpg	634.88	J/mol×K	763.86	Joback Method
cpg	647.03	J/mol×K	793.45	Joback Method
cpg	658.50	J/mol×K	823.05	Joback Method

Sources

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=U370859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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