Diethylmalonic acid, decyl 2-fluoroethyl ester

Inchi: InChI=1S/C19H35FO4/c1-4-7-8-9-10-11-12-13-15-23-17(21)19(5-2,6-3)18(22)24-16-14-2
InchiKey: AQWFZZCMLGQHGV-UHFFFAOYSA-N
Formula: C19H35FO4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 346.48

Physical Properties

Property code	Value	Unit	Source
gf	-550.71	kJ/mol	Joback Method
hf	-1129.95	kJ/mol	Joback Method
hfus	46.21	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.989		Crippen Method
mcvol	295.220	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	782.74	K	Joback Method
tc	963.60	K	Joback Method
tf	451.22	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.68	J/mol×K	782.74	Joback Method
cpg	935.20	J/mol×K	812.88	Joback Method
cpg	951.74	J/mol×K	843.03	Joback Method
cpg	967.32	J/mol×K	873.17	Joback Method
cpg	981.99	J/mol×K	903.32	Joback Method
cpg	995.76	J/mol×K	933.46	Joback Method
cpg	1008.67	J/mol×K	963.60	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370864&Units=SI

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