Diethylmalonic acid, 2-fluoroethyl undecyl ester

Inchi: InChI=1S/C20H37FO4/c1-4-7-8-9-10-11-12-13-14-16-24-18(22)20(5-2,6-3)19(23)25-17-1

InchiKey: FEJQOLQFHVNDHO-UHFFFAOYSA-N

Formula: C20H37FO4

SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF

Mol. weight [g/mol]: 360.50

Physical Properties

Property code	Value	Unit	Source
gf	-542.29	kJ/mol	Joback Method
hf	-1150.59	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	76.31	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	5.380		Crippen Method
mcvol	309.310	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	2152.00		NIST Webbook
tb	805.62	K	Joback Method
tc	989.12	K	Joback Method
tf	462.49	K	Joback Method
vc	1.210	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.61	J/mol×K	805.62	Joback Method
cpg	995.52	J/mol×K	836.20	Joback Method
cpg	1012.41	J/mol×K	866.79	Joback Method
cpg	1028.30	J/mol×K	897.37	Joback Method
cpg	1043.22	J/mol×K	927.95	Joback Method
cpg	1057.21	J/mol×K	958.54	Joback Method
cpg	1070.28	J/mol×K	989.12	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=U370865&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