Diethylmalonic acid, dodecyl 2-fluoroethyl ester

Inchi: InChI=1S/C21H39FO4/c1-4-7-8-9-10-11-12-13-14-15-17-25-19(23)21(5-2,6-3)20(24)26-1
InchiKey: ODTKMUXKPSWKQP-UHFFFAOYSA-N
Formula: C21H39FO4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 374.53

Physical Properties

Property code	Value	Unit	Source
gf	-533.87	kJ/mol	Joback Method
hf	-1171.23	kJ/mol	Joback Method
hfus	51.39	kJ/mol	Joback Method
hvap	78.54	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.770		Crippen Method
mcvol	323.400	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	2255.00		NIST Webbook
tb	828.50	K	Joback Method
tc	1015.38	K	Joback Method
tf	473.76	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.34	J/mol×K	828.50	Joback Method
cpg	1056.68	J/mol×K	859.65	Joback Method
cpg	1073.93	J/mol×K	890.79	Joback Method
cpg	1090.13	J/mol×K	921.94	Joback Method
cpg	1105.31	J/mol×K	953.09	Joback Method
cpg	1119.50	J/mol×K	984.24	Joback Method
cpg	1132.74	J/mol×K	1015.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370866&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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