Diethylmalonic acid, 2-fluoroethyl heptyl ester

Inchi: InChI=1S/C16H29FO4/c1-4-7-8-9-10-12-20-14(18)16(5-2,6-3)15(19)21-13-11-17/h4-13H
InchiKey: BWMLKJKQFYKIEJ-UHFFFAOYSA-N
Formula: C16H29FO4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 304.40

Physical Properties

Property code	Value	Unit	Source
gf	-575.97	kJ/mol	Joback Method
hf	-1068.03	kJ/mol	Joback Method
hfus	38.44	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.819		Crippen Method
mcvol	252.950	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	714.10	K	Joback Method
tc	890.98	K	Joback Method
tf	417.41	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.45	J/mol×K	714.10	Joback Method
cpg	759.80	J/mol×K	743.58	Joback Method
cpg	775.29	J/mol×K	773.06	Joback Method
cpg	789.96	J/mol×K	802.54	Joback Method
cpg	803.82	J/mol×K	832.02	Joback Method
cpg	816.90	J/mol×K	861.50	Joback Method
cpg	829.20	J/mol×K	890.98	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=U370862&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

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