Diethylmalonic acid, 2-fluoroethyl octyl ester

Inchi: InChI=1S/C17H31FO4/c1-4-7-8-9-10-11-13-21-15(19)17(5-2,6-3)16(20)22-14-12-18/h4-1
InchiKey: MWTWOOOPLAKQFV-UHFFFAOYSA-N
Formula: C17H31FO4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCF
Mol. weight [g/mol]: 318.42

Physical Properties

Property code	Value	Unit	Source
gf	-567.55	kJ/mol	Joback Method
hf	-1088.67	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	69.63	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	4.209		Crippen Method
mcvol	267.040	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	1856.00		NIST Webbook
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tb	736.98	K	Joback Method
tc	914.59	K	Joback Method
tf	428.68	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	800.53	J/mol×K	736.98	Joback Method
cpg	817.27	J/mol×K	766.58	Joback Method
cpg	833.12	J/mol×K	796.18	Joback Method
cpg	848.10	J/mol×K	825.79	Joback Method
cpg	862.25	J/mol×K	855.39	Joback Method
cpg	875.57	J/mol×K	884.99	Joback Method
cpg	888.09	J/mol×K	914.59	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=U370863&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