Diethylmalonic acid, 2-fluorophenyl octyl ester

Inchi: InChI=1S/C21H31FO4/c1-4-7-8-9-10-13-16-25-19(23)21(5-2,6-3)20(24)26-18-15-12-11-1
InchiKey: VVOOXCSQTAHHDS-UHFFFAOYSA-N
Formula: C21H31FO4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1F
Mol. weight [g/mol]: 366.47

Physical Properties

Property code	Value	Unit	Source
gf	-431.09	kJ/mol	Joback Method
hf	-946.17	kJ/mol	Joback Method
hfus	45.04	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.441		Crippen Method
mcvol	299.640	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	860.16	K	Joback Method
tc	1061.67	K	Joback Method
tf	512.70	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.22	J/mol×K	860.16	Joback Method
cpg	961.27	J/mol×K	893.74	Joback Method
cpg	976.18	J/mol×K	927.33	Joback Method
cpg	989.99	J/mol×K	960.91	Joback Method
cpg	1002.76	J/mol×K	994.50	Joback Method
cpg	1014.51	J/mol×K	1028.08	Joback Method
cpg	1025.30	J/mol×K	1061.67	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=U370132&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