Diethylmalonic acid, 2-fluorophenyl isobutyl ester

Inchi: InChI=1S/C17H23FO4/c1-5-17(6-2,15(19)21-11-12(3)4)16(20)22-14-10-8-7-9-13(14)18/h

InchiKey: WTLLIUHLZGKJHU-UHFFFAOYSA-N

Formula: C17H23FO4

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccccc1F

Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-467.21	kJ/mol	Joback Method
hf	-868.89	kJ/mol	Joback Method
hfus	31.15	kJ/mol	Joback Method
hvap	72.19	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.737		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	768.20	K	Joback Method
tc	972.60	K	Joback Method
tf	452.62	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.41	J/mol×K	768.20	Joback Method
cpg	729.75	J/mol×K	802.27	Joback Method
cpg	744.04	J/mol×K	836.33	Joback Method
cpg	757.30	J/mol×K	870.40	Joback Method
cpg	769.56	J/mol×K	904.46	Joback Method
cpg	780.86	J/mol×K	938.53	Joback Method
cpg	791.23	J/mol×K	972.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370127&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