Diethylmalonic acid, butyl 3-fluorophenyl ester

Inchi: InChI=1S/C17H23FO4/c1-4-7-11-21-15(19)17(5-2,6-3)16(20)22-14-10-8-9-13(18)12-14/h
InchiKey: GYPVHDOAFGPXMA-UHFFFAOYSA-N
Formula: C17H23FO4
SMILES: CCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 310.36

Physical Properties

Property code	Value	Unit	Source
gf	-464.77	kJ/mol	Joback Method
hf	-863.61	kJ/mol	Joback Method
hfus	34.68	kJ/mol	Joback Method
hvap	72.57	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.881		Crippen Method
mcvol	243.280	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	1854.00		NIST Webbook
tb	768.64	K	Joback Method
tc	970.27	K	Joback Method
tf	467.62	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	713.86	J/mol×K	768.64	Joback Method
cpg	729.00	J/mol×K	802.25	Joback Method
cpg	743.11	J/mol×K	835.85	Joback Method
cpg	756.23	J/mol×K	869.46	Joback Method
cpg	768.39	J/mol×K	903.06	Joback Method
cpg	779.62	J/mol×K	936.67	Joback Method
cpg	789.96	J/mol×K	970.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370198&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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