Diethylmalonic acid, 3-fluorophenyl propyl ester

Inchi: InChI=1S/C16H21FO4/c1-4-10-20-14(18)16(5-2,6-3)15(19)21-13-9-7-8-12(17)11-13/h7-9

InchiKey: RPLZZJQQHCYGLT-UHFFFAOYSA-N

Formula: C16H21FO4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 296.33

Physical Properties

Property code	Value	Unit	Source
gf	-473.19	kJ/mol	Joback Method
hf	-842.97	kJ/mol	Joback Method
hfus	32.09	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.491		Crippen Method
mcvol	229.190	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	1778.00		NIST Webbook
rinpol	1778.00		NIST Webbook
tb	745.76	K	Joback Method
tc	948.92	K	Joback Method
tf	456.35	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.33	J/mol×K	745.76	Joback Method
cpg	673.19	J/mol×K	779.62	Joback Method
cpg	687.05	J/mol×K	813.48	Joback Method
cpg	699.93	J/mol×K	847.34	Joback Method
cpg	711.88	J/mol×K	881.20	Joback Method
cpg	722.92	J/mol×K	915.06	Joback Method
cpg	733.07	J/mol×K	948.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370196&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

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