Dimethylmalonic acid, butyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C16H18F4O4/c1-4-5-9-23-13(21)15(2,3)14(22)24-11-8-6-7-10(12(11)17)16(18

InchiKey: VITMTXJMHODUFD-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1064.41	kJ/mol	Joback Method
hf	-1451.52	kJ/mol	Joback Method
hfus	33.52	kJ/mol	Joback Method
hvap	67.26	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.119		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	745.32	K	Joback Method
tc	937.83	K	Joback Method
tf	473.06	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	682.92	J/mol×K	745.32	Joback Method
cpg	696.34	J/mol×K	777.41	Joback Method
cpg	708.85	J/mol×K	809.49	Joback Method
cpg	720.48	J/mol×K	841.58	Joback Method
cpg	731.28	J/mol×K	873.66	Joback Method
cpg	741.28	J/mol×K	905.75	Joback Method
cpg	750.53	J/mol×K	937.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361996&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