Dimethylmalonic acid, butyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C15H17F3O4/c1-4-5-8-21-13(19)15(2,3)14(20)22-10-7-6-9(16)11(17)12(10)18

InchiKey: MFYQGRFBTUIZGZ-UHFFFAOYSA-N

Formula: C15H17F3O4

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-890.49	kJ/mol	Joback Method
hf	-1237.49	kJ/mol	Joback Method
hfus	34.88	kJ/mol	Joback Method
hvap	67.81	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.379		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	1670.00		NIST Webbook
tb	731.38	K	Joback Method
tc	924.50	K	Joback Method
tf	471.30	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.67	J/mol×K	731.38	Joback Method
cpg	630.86	J/mol×K	763.57	Joback Method
cpg	643.23	J/mol×K	795.75	Joback Method
cpg	654.77	J/mol×K	827.94	Joback Method
cpg	665.51	J/mol×K	860.13	Joback Method
cpg	675.47	J/mol×K	892.31	Joback Method
cpg	684.65	J/mol×K	924.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361882&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