Dimethylmalonic acid, butyl 3,5-difluorophenyl ester

Inchi: InChI=1S/C15H18F2O4/c1-4-5-6-20-13(18)15(2,3)14(19)21-12-8-10(16)7-11(17)9-12/h7-

InchiKey: WTLCPKVMKGYPCF-UHFFFAOYSA-N

Formula: C15H18F2O4

SMILES: CCCCOC(=O)C(C)(C)C(=O)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 300.30

Physical Properties

Property code	Value	Unit	Source
gf	-686.05	kJ/mol	Joback Method
hf	-1029.91	kJ/mol	Joback Method
hfus	32.19	kJ/mol	Joback Method
hvap	67.97	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.240		Crippen Method
mcvol	216.870	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	1621.00		NIST Webbook
rinpol	1621.00		NIST Webbook
tb	727.13	K	Joback Method
tc	925.93	K	Joback Method
tf	458.19	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.80	J/mol×K	727.13	Joback Method
cpg	624.63	J/mol×K	760.26	Joback Method
cpg	637.57	J/mol×K	793.40	Joback Method
cpg	649.62	J/mol×K	826.53	Joback Method
cpg	660.82	J/mol×K	859.66	Joback Method
cpg	671.18	J/mol×K	892.79	Joback Method
cpg	680.73	J/mol×K	925.93	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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