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

Inchi: InChI=1S/C18H22F4O4/c1-4-7-11-25-15(23)17(5-2,6-3)16(24)26-13-10-8-9-12(14(13)19)18(20,21)22/h8-10H,4-7,11H2,1-3H3

InchiKey: FRPQXLSHSUMHID-UHFFFAOYSA-N

Formula: C18H22F4O4

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

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1047.57	kJ/mol	Joback Method
hf	-1492.80	kJ/mol	Joback Method
hfus	38.70	kJ/mol	Joback Method
hvap	71.71	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.900		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1376.84	kPa	Joback Method
rinpol	1824.00		NIST Webbook
rinpol	1824.00		NIST Webbook
tb	791.08	K	Joback Method
tc	983.28	K	Joback Method
tf	495.60	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.96	J/mol×K	791.08	Joback Method
cpg	808.02	J/mol×K	823.11	Joback Method
cpg	821.13	J/mol×K	855.15	Joback Method
cpg	833.32	J/mol×K	887.18	Joback Method
cpg	844.64	J/mol×K	919.22	Joback Method
cpg	855.14	J/mol×K	951.25	Joback Method
cpg	864.85	J/mol×K	983.28	Joback Method

Sources

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=U370710&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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