Diethylmalonic acid, butyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C14H23F3O4/c1-5-8-9-20-11(18)13(6-2,7-3)12(19)21-10(4)14(15,16)17/h10H,

InchiKey: CTIJGIQDHWXBQD-UHFFFAOYSA-N

Formula: C14H23F3O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 312.33

Physical Properties

Property code	Value	Unit	Source
gf	-982.03	kJ/mol	Joback Method
hf	-1433.00	kJ/mol	Joback Method
hfus	28.48	kJ/mol	Joback Method
hvap	59.64	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.630		Crippen Method
mcvol	228.310	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1336.00		NIST Webbook
tb	663.21	K	Joback Method
tc	837.85	K	Joback Method
tf	383.47	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.64	J/mol×K	663.21	Joback Method
cpg	666.72	J/mol×K	692.32	Joback Method
cpg	680.97	J/mol×K	721.42	Joback Method
cpg	694.44	J/mol×K	750.53	Joback Method
cpg	707.13	J/mol×K	779.64	Joback Method
cpg	719.10	J/mol×K	808.75	Joback Method
cpg	730.35	J/mol×K	837.85	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=U370816&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