Dimethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl pentyl ester

Inchi: InChI=1S/C13H20BrF3O4/c1-4-5-6-7-20-10(18)12(2,3)11(19)21-9(8-14)13(15,16)17/h9H

InchiKey: NGELFJQIEDGPAB-UHFFFAOYSA-N

Formula: C13H20BrF3O4

SMILES: CCCCCOC(=O)C(C)(C)C(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 377.19

Physical Properties

Property code	Value	Unit	Source
gf	-976.13	kJ/mol	Joback Method
hf	-1386.03	kJ/mol	Joback Method
hfus	31.17	kJ/mol	Joback Method
hvap	63.85	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.615		Crippen Method
mcvol	231.720	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	1532.00		NIST Webbook
tb	706.49	K	Joback Method
tc	892.82	K	Joback Method
tf	432.00	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.06	J/mol×K	706.49	Joback Method
cpg	655.38	J/mol×K	737.54	Joback Method
cpg	667.87	J/mol×K	768.60	Joback Method
cpg	679.58	J/mol×K	799.65	Joback Method
cpg	690.54	J/mol×K	830.71	Joback Method
cpg	700.80	J/mol×K	861.76	Joback Method
cpg	710.38	J/mol×K	892.82	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=U361930&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