Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl tridecyl ester

Inchi: InChI=1S/C23H40BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-30-20(28)22(5-2,6-3)21(2

InchiKey: KQPRIUMKGPMEGV-UHFFFAOYSA-N

Formula: C23H40BrF3O4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 517.46

Physical Properties

Property code	Value	Unit	Source
gf	-891.93	kJ/mol	Joback Method
hf	-1592.43	kJ/mol	Joback Method
hfus	57.07	kJ/mol	Joback Method
hvap	86.11	kJ/mol	Joback Method
log10ws	-8.14		Crippen Method
logp	7.516		Crippen Method
mcvol	372.620	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2443.00		NIST Webbook
rinpol	2443.00		NIST Webbook
tb	935.29	K	Joback Method
tc	1146.26	K	Joback Method
tf	544.70	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1223.38	J/mol×K	935.29	Joback Method
cpg	1240.91	J/mol×K	970.45	Joback Method
cpg	1257.25	J/mol×K	1005.61	Joback Method
cpg	1272.50	J/mol×K	1040.78	Joback Method
cpg	1286.74	J/mol×K	1075.94	Joback Method
cpg	1300.05	J/mol×K	1111.10	Joback Method
cpg	1312.53	J/mol×K	1146.26	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370805&Units=SI

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