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

Inchi: InChI=1S/C20H34BrF3O4/c1-4-7-8-9-10-11-12-13-14-27-17(25)19(5-2,6-3)18(26)28-16(1

InchiKey: YSCMQYLPUACKGU-UHFFFAOYSA-N

Formula: C20H34BrF3O4

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

Mol. weight [g/mol]: 475.38

Physical Properties

Property code	Value	Unit	Source
gf	-917.19	kJ/mol	Joback Method
hf	-1530.51	kJ/mol	Joback Method
hfus	49.30	kJ/mol	Joback Method
hvap	79.43	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.346		Crippen Method
mcvol	330.350	ml/mol	McGowan Method
pc	1063.79	kPa	Joback Method
rinpol	2130.00		NIST Webbook
tb	866.65	K	Joback Method
tc	1062.00	K	Joback Method
tf	510.89	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.52	J/mol×K	866.65	Joback Method
cpg	1056.54	J/mol×K	899.21	Joback Method
cpg	1071.54	J/mol×K	931.77	Joback Method
cpg	1085.58	J/mol×K	964.32	Joback Method
cpg	1098.73	J/mol×K	996.88	Joback Method
cpg	1111.04	J/mol×K	1029.44	Joback Method
cpg	1122.57	J/mol×K	1062.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370802&Units=SI
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

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