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

Inchi: InChI=1S/C28H50BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-35-25(33
InchiKey: RETBGVOFZDGUEA-UHFFFAOYSA-N
Formula: C28H50BrF3O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 587.59

Physical Properties

Property code	Value	Unit	Source
gf	-849.83	kJ/mol	Joback Method
hf	-1695.63	kJ/mol	Joback Method
hfus	70.02	kJ/mol	Joback Method
hvap	97.24	kJ/mol	Joback Method
log10ws	-10.23		Crippen Method
logp	9.467		Crippen Method
mcvol	443.070	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	2953.00		NIST Webbook
rinpol	2953.00		NIST Webbook
tb	1049.69	K	Joback Method
tc	1309.69	K	Joback Method
tf	601.05	K	Joback Method
vc	1.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.37	J/mol×K	1049.69	Joback Method
cpg	1560.70	J/mol×K	1093.02	Joback Method
cpg	1580.39	J/mol×K	1136.36	Joback Method
cpg	1598.65	J/mol×K	1179.69	Joback Method
cpg	1615.66	J/mol×K	1223.02	Joback Method
cpg	1631.61	J/mol×K	1266.36	Joback Method
cpg	1646.70	J/mol×K	1309.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370810&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

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