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

Inchi: InChI=1S/C27H48BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-34-24(32)26
InchiKey: YEJASGVQVYXWOT-UHFFFAOYSA-N
Formula: C27H48BrF3O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 573.57

Physical Properties

Property code	Value	Unit	Source
gf	-858.25	kJ/mol	Joback Method
hf	-1674.99	kJ/mol	Joback Method
hfus	67.43	kJ/mol	Joback Method
hvap	95.01	kJ/mol	Joback Method
log10ws	-9.81		Crippen Method
logp	9.076		Crippen Method
mcvol	428.980	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	2837.00		NIST Webbook
rinpol	2837.00		NIST Webbook
tb	1026.81	K	Joback Method
tc	1274.27	K	Joback Method
tf	589.78	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1475.23	J/mol×K	1026.81	Joback Method
cpg	1495.62	J/mol×K	1068.05	Joback Method
cpg	1514.50	J/mol×K	1109.30	Joback Method
cpg	1532.01	J/mol×K	1150.54	Joback Method
cpg	1548.33	J/mol×K	1191.78	Joback Method
cpg	1563.60	J/mol×K	1233.03	Joback Method
cpg	1577.99	J/mol×K	1274.27	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=U370809&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