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

Inchi: InChI=1S/C25H44BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-32-22(30)24(5-2,6

InchiKey: LPYULUAJEHVLFF-UHFFFAOYSA-N

Formula: C25H44BrF3O4

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

Mol. weight [g/mol]: 545.51

Physical Properties

Property code	Value	Unit	Source
gf	-875.09	kJ/mol	Joback Method
hf	-1633.71	kJ/mol	Joback Method
hfus	62.25	kJ/mol	Joback Method
hvap	90.56	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.296		Crippen Method
mcvol	400.800	ml/mol	McGowan Method
pc	795.28	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	981.05	K	Joback Method
tc	1207.74	K	Joback Method
tf	567.24	K	Joback Method
vc	1.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.29	J/mol×K	981.05	Joback Method
cpg	1367.10	J/mol×K	1018.83	Joback Method
cpg	1384.58	J/mol×K	1056.61	Joback Method
cpg	1400.84	J/mol×K	1094.39	Joback Method
cpg	1416.00	J/mol×K	1132.18	Joback Method
cpg	1430.17	J/mol×K	1169.96	Joback Method
cpg	1443.47	J/mol×K	1207.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370807&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