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

Inchi: InChI=1S/C21H36BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-28-18(26)20(5-2,6-3)19(27)29-1

InchiKey: ZPJQCJZFULVDIK-UHFFFAOYSA-N

Formula: C21H36BrF3O4

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

Mol. weight [g/mol]: 489.41

Physical Properties

Property code	Value	Unit	Source
gf	-908.77	kJ/mol	Joback Method
hf	-1551.15	kJ/mol	Joback Method
hfus	51.89	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.736		Crippen Method
mcvol	344.440	ml/mol	McGowan Method
pc	1000.18	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	889.53	K	Joback Method
tc	1089.13	K	Joback Method
tf	522.16	K	Joback Method
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1100.81	J/mol×K	889.53	Joback Method
cpg	1117.29	J/mol×K	922.80	Joback Method
cpg	1132.70	J/mol×K	956.06	Joback Method
cpg	1147.11	J/mol×K	989.33	Joback Method
cpg	1160.59	J/mol×K	1022.60	Joback Method
cpg	1173.21	J/mol×K	1055.86	Joback Method
cpg	1185.03	J/mol×K	1089.13	Joback Method

Sources

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=U370803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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