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

Inchi: InChI=1S/C19H32BrF3O4/c1-4-7-8-9-10-11-12-13-26-16(24)18(5-2,6-3)17(25)27-15(14-2
InchiKey: OIIGMPVTPDFKGL-UHFFFAOYSA-N
Formula: C19H32BrF3O4
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F
Mol. weight [g/mol]: 461.35

Physical Properties

Property code	Value	Unit	Source
gf	-925.61	kJ/mol	Joback Method
hf	-1509.87	kJ/mol	Joback Method
hfus	46.71	kJ/mol	Joback Method
hvap	77.20	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.956		Crippen Method
mcvol	316.260	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2038.00		NIST Webbook
tb	843.77	K	Joback Method
tc	1035.73	K	Joback Method
tf	499.62	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.95	J/mol×K	843.77	Joback Method
cpg	996.55	J/mol×K	875.76	Joback Method
cpg	1011.17	J/mol×K	907.76	Joback Method
cpg	1024.87	J/mol×K	939.75	Joback Method
cpg	1037.70	J/mol×K	971.74	Joback Method
cpg	1049.71	J/mol×K	1003.74	Joback Method
cpg	1060.97	J/mol×K	1035.73	Joback Method

Sources

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=U370801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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