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

Inchi: InChI=1S/C21H37F3O4/c1-5-8-9-10-11-12-13-14-15-16-27-18(25)20(6-2,7-3)19(26)28-1
InchiKey: DNEMOOHWOXBQMO-UHFFFAOYSA-N
Formula: C21H37F3O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 410.51

Physical Properties

Property code	Value	Unit	Source
gf	-923.09	kJ/mol	Joback Method
hf	-1577.48	kJ/mol	Joback Method
hfus	46.61	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.361		Crippen Method
mcvol	326.940	ml/mol	McGowan Method
pc	957.91	kPa	Joback Method
rinpol	1997.00		NIST Webbook
rinpol	1997.00		NIST Webbook
tb	823.37	K	Joback Method
tc	1008.91	K	Joback Method
tf	462.36	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.35	J/mol×K	823.37	Joback Method
cpg	1072.16	J/mol×K	854.29	Joback Method
cpg	1088.90	J/mol×K	885.22	Joback Method
cpg	1104.62	J/mol×K	916.14	Joback Method
cpg	1119.36	J/mol×K	947.06	Joback Method
cpg	1133.17	J/mol×K	977.99	Joback Method
cpg	1146.10	J/mol×K	1008.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370821&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