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

Inchi: InChI=1S/C28H51F3O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-34-25(32)
InchiKey: RYCOYJIUHQOPRJ-UHFFFAOYSA-N
Formula: C28H51F3O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 508.70

Physical Properties

Property code	Value	Unit	Source
gf	-864.15	kJ/mol	Joback Method
hf	-1721.96	kJ/mol	Joback Method
hfus	64.74	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.091		Crippen Method
mcvol	425.570	ml/mol	McGowan Method
pc	656.45	kPa	Joback Method
rinpol	2696.00		NIST Webbook
rinpol	2696.00		NIST Webbook
tb	983.53	K	Joback Method
tc	1220.82	K	Joback Method
tf	541.25	K	Joback Method
vc	1.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1494.13	J/mol×K	983.53	Joback Method
cpg	1516.35	J/mol×K	1023.08	Joback Method
cpg	1536.86	J/mol×K	1062.63	Joback Method
cpg	1555.79	J/mol×K	1102.17	Joback Method
cpg	1573.27	J/mol×K	1141.72	Joback Method
cpg	1589.42	J/mol×K	1181.27	Joback Method
cpg	1604.39	J/mol×K	1220.82	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=U370828&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