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

Inchi: InChI=1S/C20H35F3O4/c1-5-8-9-10-11-12-13-14-15-26-17(24)19(6-2,7-3)18(25)27-16(4
InchiKey: JAMOXBZTNAPWNM-UHFFFAOYSA-N
Formula: C20H35F3O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 396.48

Physical Properties

Property code	Value	Unit	Source
gf	-931.51	kJ/mol	Joback Method
hf	-1556.84	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.971		Crippen Method
mcvol	312.850	ml/mol	McGowan Method
pc	1017.48	kPa	Joback Method
rinpol	1893.00		NIST Webbook
tb	800.49	K	Joback Method
tc	982.51	K	Joback Method
tf	451.09	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.07	J/mol×K	800.49	Joback Method
cpg	1011.45	J/mol×K	830.83	Joback Method
cpg	1027.81	J/mol×K	861.16	Joback Method
cpg	1043.20	J/mol×K	891.50	Joback Method
cpg	1057.65	J/mol×K	921.84	Joback Method
cpg	1071.20	J/mol×K	952.18	Joback Method
cpg	1083.91	J/mol×K	982.51	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370820&Units=SI

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