Diethylmalonic acid, 2,2,3,3,4,4,4-heptafluorobutyl nonyl ester

Inchi: InChI=1S/C20H31F7O4/c1-4-7-8-9-10-11-12-13-30-15(28)17(5-2,6-3)16(29)31-14-18(21

InchiKey: FLQJOVAAKXGLPP-UHFFFAOYSA-N

Formula: C20H31F7O4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 468.45

Physical Properties

Property code	Value	Unit	Source
gf	-1702.63	kJ/mol	Joback Method
hf	-2353.50	kJ/mol	Joback Method
hfus	45.03	kJ/mol	Joback Method
hvap	67.52	kJ/mol	Joback Method
log10ws	-6.97		Crippen Method
logp	6.463		Crippen Method
mcvol	319.930	ml/mol	McGowan Method
pc	926.68	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	791.55	K	Joback Method
tc	969.47	K	Joback Method
tf	473.29	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.97	J/mol×K	791.55	Joback Method
cpg	1042.19	J/mol×K	821.20	Joback Method
cpg	1057.42	J/mol×K	850.86	Joback Method
cpg	1071.75	J/mol×K	880.51	Joback Method
cpg	1085.22	J/mol×K	910.16	Joback Method
cpg	1097.91	J/mol×K	939.82	Joback Method
cpg	1109.89	J/mol×K	969.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368434&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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