Diethylmalonic acid, 2,2,3,3,4,4,5,5-octafluoropentyl heptyl ester

Inchi: InChI=1S/C19H28F8O4/c1-4-7-8-9-10-11-30-14(28)16(5-2,6-3)15(29)31-12-17(22,23)19

InchiKey: RKWUIKQTYDSOFR-UHFFFAOYSA-N

Formula: C19H28F8O4

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

Mol. weight [g/mol]: 472.41

Physical Properties

Property code	Value	Unit	Source
gf	-1908.30	kJ/mol	Joback Method
hf	-2534.25	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	64.09	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	6.021		Crippen Method
mcvol	307.610	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	1741.00		NIST Webbook
tb	767.50	K	Joback Method
tc	940.57	K	Joback Method
tf	447.61	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.47	J/mol×K	767.50	Joback Method
cpg	991.06	J/mol×K	796.35	Joback Method
cpg	1005.70	J/mol×K	825.19	Joback Method
cpg	1019.45	J/mol×K	854.04	Joback Method
cpg	1032.37	J/mol×K	882.88	Joback Method
cpg	1044.52	J/mol×K	911.73	Joback Method
cpg	1055.97	J/mol×K	940.57	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370655&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