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

Inchi: InChI=1S/C20H30F8O4/c1-4-7-8-9-10-11-12-31-15(29)17(5-2,6-3)16(30)32-13-18(23,24)

InchiKey: AIFCCBPVAVCKCN-UHFFFAOYSA-N

Formula: C20H30F8O4

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

Mol. weight [g/mol]: 486.44

Physical Properties

Property code	Value	Unit	Source
gf	-1899.88	kJ/mol	Joback Method
hf	-2554.89	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	66.32	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.411		Crippen Method
mcvol	321.700	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	1829.00		NIST Webbook
rinpol	1829.00		NIST Webbook
tb	790.38	K	Joback Method
tc	967.76	K	Joback Method
tf	458.88	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.99	J/mol×K	790.38	Joback Method
cpg	1050.08	J/mol×K	819.94	Joback Method
cpg	1065.18	J/mol×K	849.51	Joback Method
cpg	1079.36	J/mol×K	879.07	Joback Method
cpg	1092.68	J/mol×K	908.63	Joback Method
cpg	1105.21	J/mol×K	938.19	Joback Method
cpg	1117.02	J/mol×K	967.76	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=U370656&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