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

Inchi: InChI=1S/C18H26F8O4/c1-4-7-8-9-10-29-13(27)15(5-2,6-3)14(28)30-11-16(21,22)18(25

InchiKey: QJZLXYBPDZMJBW-UHFFFAOYSA-N

Formula: C18H26F8O4

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

Mol. weight [g/mol]: 458.38

Physical Properties

Property code	Value	Unit	Source
gf	-1916.72	kJ/mol	Joback Method
hf	-2513.61	kJ/mol	Joback Method
hfus	39.41	kJ/mol	Joback Method
hvap	61.87	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.630		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1020.73	kPa	Joback Method
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
tb	744.62	K	Joback Method
tc	914.14	K	Joback Method
tf	436.34	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	917.81	J/mol×K	744.62	Joback Method
cpg	932.94	J/mol×K	772.87	Joback Method
cpg	947.15	J/mol×K	801.13	Joback Method
cpg	960.50	J/mol×K	829.38	Joback Method
cpg	973.04	J/mol×K	857.63	Joback Method
cpg	984.84	J/mol×K	885.89	Joback Method
cpg	995.94	J/mol×K	914.14	Joback Method

Sources

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=U370654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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