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

Inchi: InChI=1S/C19H29F7O4/c1-4-7-8-9-10-11-12-29-14(27)16(5-2,6-3)15(28)30-13-17(20,21)

InchiKey: YVNZYVKZCKJCQZ-UHFFFAOYSA-N

Formula: C19H29F7O4

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

Mol. weight [g/mol]: 454.42

Physical Properties

Property code	Value	Unit	Source
gf	-1711.05	kJ/mol	Joback Method
hf	-2332.86	kJ/mol	Joback Method
hfus	42.44	kJ/mol	Joback Method
hvap	65.30	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	6.073		Crippen Method
mcvol	305.840	ml/mol	McGowan Method
pc	983.31	kPa	Joback Method
rinpol	1723.00		NIST Webbook
rinpol	1723.00		NIST Webbook
tb	768.67	K	Joback Method
tc	942.66	K	Joback Method
tf	462.02	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.37	J/mol×K	768.67	Joback Method
cpg	983.11	J/mol×K	797.67	Joback Method
cpg	997.90	J/mol×K	826.67	Joback Method
cpg	1011.80	J/mol×K	855.66	Joback Method
cpg	1024.88	J/mol×K	884.66	Joback Method
cpg	1037.20	J/mol×K	913.66	Joback Method
cpg	1048.82	J/mol×K	942.66	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=U368433&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

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