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

Inchi: InChI=1S/C18H27F7O4/c1-4-7-8-9-10-11-28-13(26)15(5-2,6-3)14(27)29-12-16(19,20)17

InchiKey: BGICUZPKOFZWII-UHFFFAOYSA-N

Formula: C18H27F7O4

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

Mol. weight [g/mol]: 440.39

Physical Properties

Property code	Value	Unit	Source
gf	-1719.47	kJ/mol	Joback Method
hf	-2312.22	kJ/mol	Joback Method
hfus	39.85	kJ/mol	Joback Method
hvap	63.07	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.683		Crippen Method
mcvol	291.750	ml/mol	McGowan Method
pc	1045.30	kPa	Joback Method
rinpol	1632.00		NIST Webbook
tb	745.79	K	Joback Method
tc	916.58	K	Joback Method
tf	450.75	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.63	J/mol×K	745.79	Joback Method
cpg	924.92	J/mol×K	774.25	Joback Method
cpg	939.30	J/mol×K	802.72	Joback Method
cpg	952.81	J/mol×K	831.18	Joback Method
cpg	965.53	J/mol×K	859.65	Joback Method
cpg	977.50	J/mol×K	888.11	Joback Method
cpg	988.77	J/mol×K	916.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368432&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