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

Inchi: InChI=1S/C16H23F7O4/c1-4-7-8-9-26-11(24)13(5-2,6-3)12(25)27-10-14(17,18)15(19,20)

InchiKey: YZGBCYPTABMUCY-UHFFFAOYSA-N

Formula: C16H23F7O4

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

Mol. weight [g/mol]: 412.34

Physical Properties

Property code	Value	Unit	Source
gf	-1736.31	kJ/mol	Joback Method
hf	-2270.94	kJ/mol	Joback Method
hfus	34.67	kJ/mol	Joback Method
hvap	58.62	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.902		Crippen Method
mcvol	263.570	ml/mol	McGowan Method
pc	1188.24	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
tb	700.03	K	Joback Method
tc	866.37	K	Joback Method
tf	428.21	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.96	J/mol×K	700.03	Joback Method
cpg	811.44	J/mol×K	727.75	Joback Method
cpg	825.05	J/mol×K	755.48	Joback Method
cpg	837.85	J/mol×K	783.20	Joback Method
cpg	849.88	J/mol×K	810.92	Joback Method
cpg	861.18	J/mol×K	838.64	Joback Method
cpg	871.82	J/mol×K	866.37	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=U368430&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