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

Inchi: InChI=1S/C28H47F7O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-38-23(36)25(5

InchiKey: GXJOTEMWFIGBEG-UHFFFAOYSA-N

Formula: C28H47F7O4

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

Mol. weight [g/mol]: 580.66

Physical Properties

Property code	Value	Unit	Source
gf	-1635.27	kJ/mol	Joback Method
hf	-2518.62	kJ/mol	Joback Method
hfus	65.75	kJ/mol	Joback Method
hvap	85.33	kJ/mol	Joback Method
log10ws	-10.32		Crippen Method
logp	9.584		Crippen Method
mcvol	432.650	ml/mol	McGowan Method
pc	608.76	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	974.59	K	Joback Method
tc	1219.58	K	Joback Method
tf	563.45	K	Joback Method
vc	1.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.07	J/mol×K	974.59	Joback Method
cpg	1542.60	J/mol×K	1015.42	Joback Method
cpg	1563.61	J/mol×K	1056.25	Joback Method
cpg	1583.31	J/mol×K	1097.09	Joback Method
cpg	1601.93	J/mol×K	1137.92	Joback Method
cpg	1619.67	J/mol×K	1178.75	Joback Method
cpg	1636.75	J/mol×K	1219.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368442&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