Dodecanoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C17H26F8O2/c1-2-3-4-5-6-7-8-9-10-11-13(26)27-12-15(20,21)17(24,25)16(22

InchiKey: FYEGKTFMMKLXIW-UHFFFAOYSA-N

Formula: C17H26F8O2

SMILES: CCCCCCCCCCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 414.37

Physical Properties

Property code	Value	Unit	Source
gf	-1694.06	kJ/mol	Joback Method
hf	-2239.42	kJ/mol	Joback Method
hfus	41.45	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	6.622		Crippen Method
mcvol	271.990	ml/mol	McGowan Method
pc	1041.25	kPa	Joback Method
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
tb	648.68	K	Joback Method
tc	800.50	K	Joback Method
tf	350.49	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.46	J/mol×K	648.68	Joback Method
cpg	818.50	J/mol×K	673.98	Joback Method
cpg	833.72	J/mol×K	699.29	Joback Method
cpg	848.16	J/mol×K	724.59	Joback Method
cpg	861.86	J/mol×K	749.89	Joback Method
cpg	874.86	J/mol×K	775.20	Joback Method
cpg	887.19	J/mol×K	800.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360538&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