Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-methyl-5-methoxypentyl ester

Inchi: InChI=1S/C17H24F8O5/c1-11(6-8-28-2)7-9-29-12(26)4-3-5-13(27)30-10-15(20,21)17(24

InchiKey: XYQDKRCOUFSFAD-UHFFFAOYSA-N

Formula: C17H24F8O5

SMILES: COCCC(C)CCOC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 460.36

Physical Properties

Property code	Value	Unit	Source
gf	-2035.42	kJ/mol	Joback Method
hf	-2621.72	kJ/mol	Joback Method
hfus	41.90	kJ/mol	Joback Method
hvap	62.96	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.477		Crippen Method
mcvol	285.300	ml/mol	McGowan Method
pc	1066.57	kPa	Joback Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook
tb	746.95	K	Joback Method
tc	915.85	K	Joback Method
tf	429.88	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.93	J/mol×K	746.95	Joback Method
cpg	903.61	J/mol×K	775.10	Joback Method
cpg	917.39	J/mol×K	803.25	Joback Method
cpg	930.32	J/mol×K	831.40	Joback Method
cpg	942.44	J/mol×K	859.55	Joback Method
cpg	953.78	J/mol×K	887.70	Joback Method
cpg	964.37	J/mol×K	915.85	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393516&Units=SI

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