Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-octyl ester

Inchi: InChI=1S/C18H26F8O4/c1-3-5-6-8-12(4-2)30-14(28)10-7-9-13(27)29-11-16(21,22)18(25

InchiKey: KNLMJSVRMIPBJF-UHFFFAOYSA-N

Formula: C18H26F8O4

SMILES: CCCCCC(CC)OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 458.38

Physical Properties

Property code	Value	Unit	Source
gf	-1922.00	kJ/mol	Joback Method
hf	-2510.14	kJ/mol	Joback Method
hfus	43.30	kJ/mol	Joback Method
hvap	62.77	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.773		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook
tb	747.41	K	Joback Method
tc	916.25	K	Joback Method
tf	418.92	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.46	J/mol×K	747.41	Joback Method
cpg	931.75	J/mol×K	775.55	Joback Method
cpg	946.13	J/mol×K	803.69	Joback Method
cpg	959.65	J/mol×K	831.83	Joback Method
cpg	972.36	J/mol×K	859.97	Joback Method
cpg	984.30	J/mol×K	888.11	Joback Method
cpg	995.51	J/mol×K	916.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391554&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