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

Inchi: InChI=1S/C18H18F8O4/c1-10-5-3-6-12(11(10)2)30-14(28)8-4-7-13(27)29-9-16(21,22)18

InchiKey: VMQPBOKBZGYPPN-UHFFFAOYSA-N

Formula: C18H18F8O4

SMILES: Cc1cccc(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1C

Mol. weight [g/mol]: 450.32

Physical Properties

Property code	Value	Unit	Source
gf	-1826.41	kJ/mol	Joback Method
hf	-2291.27	kJ/mol	Joback Method
hfus	40.09	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.093		Crippen Method
mcvol	269.760	ml/mol	McGowan Method
pc	1232.88	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	784.49	K	Joback Method
tc	967.33	K	Joback Method
tf	485.38	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.70	J/mol×K	784.49	Joback Method
cpg	839.50	J/mol×K	814.96	Joback Method
cpg	851.40	J/mol×K	845.44	Joback Method
cpg	862.47	J/mol×K	875.91	Joback Method
cpg	872.74	J/mol×K	906.38	Joback Method
cpg	882.27	J/mol×K	936.86	Joback Method
cpg	891.12	J/mol×K	967.33	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=U392213&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