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

Inchi: InChI=1S/C18H18F8O4/c1-2-11-6-3-4-7-12(11)30-14(28)9-5-8-13(27)29-10-16(21,22)18
InchiKey: SFCVWSCWNCHXFQ-UHFFFAOYSA-N
Formula: C18H18F8O4
SMILES: CCc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 450.32

Physical Properties

Property code	Value	Unit	Source
gf	-1816.78	kJ/mol	Joback Method
hf	-2279.80	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.039		Crippen Method
mcvol	269.760	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	1954.00		NIST Webbook
rinpol	1954.00		NIST Webbook
tb	779.51	K	Joback Method
tc	961.43	K	Joback Method
tf	472.86	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.64	J/mol×K	779.51	Joback Method
cpg	840.54	J/mol×K	809.83	Joback Method
cpg	852.52	J/mol×K	840.15	Joback Method
cpg	863.65	J/mol×K	870.47	Joback Method
cpg	873.99	J/mol×K	900.79	Joback Method
cpg	883.59	J/mol×K	931.11	Joback Method
cpg	892.50	J/mol×K	961.43	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390849&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