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

Inchi: InChI=1S/C18H24F8O4/c1-2-11-6-3-4-7-12(11)30-14(28)9-5-8-13(27)29-10-16(21,22)18

InchiKey: YJFWHVNEBIUNSZ-UHFFFAOYSA-N

Formula: C18H24F8O4

SMILES: CCC1CCCCC1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 456.37

Physical Properties

Property code	Value	Unit	Source
gf	-1902.82	kJ/mol	Joback Method
hf	-2470.88	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	63.28	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.383		Crippen Method
mcvol	282.660	ml/mol	McGowan Method
pc	1128.35	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	762.73	K	Joback Method
tc	940.20	K	Joback Method
tf	437.06	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.25	J/mol×K	762.73	Joback Method
cpg	930.42	J/mol×K	792.31	Joback Method
cpg	945.51	J/mol×K	821.89	Joback Method
cpg	959.56	J/mol×K	851.47	Joback Method
cpg	972.63	J/mol×K	881.04	Joback Method
cpg	984.76	J/mol×K	910.62	Joback Method
cpg	996.01	J/mol×K	940.20	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=U405477&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