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

Inchi: InChI=1S/C18H26F8O4/c1-11(8-15(2,3)4)9-29-12(27)6-5-7-13(28)30-10-16(21,22)18(25

InchiKey: TWMPHXVTAWBRII-UHFFFAOYSA-N

Formula: C18H26F8O4

SMILES: CC(COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC(C)(C)C

Mol. weight [g/mol]: 458.38

Physical Properties

Property code	Value	Unit	Source
gf	-1919.16	kJ/mol	Joback Method
hf	-2518.89	kJ/mol	Joback Method
hfus	35.89	kJ/mol	Joback Method
hvap	61.48	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.486		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1025.97	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1776.00		NIST Webbook
tb	744.18	K	Joback Method
tc	914.43	K	Joback Method
tf	421.34	K	Joback Method
vc	1.179	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.31	J/mol×K	744.18	Joback Method
cpg	933.52	J/mol×K	772.56	Joback Method
cpg	947.80	J/mol×K	800.93	Joback Method
cpg	961.21	J/mol×K	829.31	Joback Method
cpg	973.79	J/mol×K	857.68	Joback Method
cpg	985.61	J/mol×K	886.06	Joback Method
cpg	996.73	J/mol×K	914.43	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=U391524&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