Glutaric acid, (2-methylcyclohex-1-enyl)methyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C18H22F8O4/c1-11-5-2-3-6-12(11)9-29-13(27)7-4-8-14(28)30-10-16(21,22)18(25,26)17(23,24)15(19)20/h15H,2-10H2,1H3

InchiKey: DRQZZPSVBZJCHI-UHFFFAOYSA-N

Formula: C18H22F8O4

SMILES: CC1=C(COC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CCCC1

Mol. weight [g/mol]: 454.35

Physical Properties

Property code	Value	Unit	Source
gf	-1876.70	kJ/mol	Joback Method
hf	-2395.36	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	65.52	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	5.305		Crippen Method
mcvol	278.360	ml/mol	McGowan Method
pc	1184.97	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	781.19	K	Joback Method
tc	962.23	K	Joback Method
tf	471.34	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	880.79	J/mol×K	781.19	Joback Method
cpg	895.24	J/mol×K	811.36	Joback Method
cpg	908.72	J/mol×K	841.54	Joback Method
cpg	921.27	J/mol×K	871.71	Joback Method
cpg	932.95	J/mol×K	901.89	Joback Method
cpg	943.81	J/mol×K	932.06	Joback Method
cpg	953.90	J/mol×K	962.23	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=U405500&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