Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C17H24F8O4/c1-4-6-11(10(2)3)29-13(27)8-5-7-12(26)28-9-15(20,21)17(24,25)

InchiKey: HZHBXTGCWLUAEV-UHFFFAOYSA-N

Formula: C17H24F8O4

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

Mol. weight [g/mol]: 444.36

Physical Properties

Property code	Value	Unit	Source
gf	-1932.86	kJ/mol	Joback Method
hf	-2494.78	kJ/mol	Joback Method
hfus	37.19	kJ/mol	Joback Method
hvap	60.16	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	5.239		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1084.20	kPa	Joback Method
rinpol	1677.00		NIST Webbook
rinpol	1677.00		NIST Webbook
tb	724.09	K	Joback Method
tc	890.30	K	Joback Method
tf	392.65	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.94	J/mol×K	724.09	Joback Method
cpg	874.83	J/mol×K	751.79	Joback Method
cpg	888.84	J/mol×K	779.49	Joback Method
cpg	902.01	J/mol×K	807.19	Joback Method
cpg	914.40	J/mol×K	834.89	Joback Method
cpg	926.02	J/mol×K	862.60	Joback Method
cpg	936.94	J/mol×K	890.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393726&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