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

Inchi: InChI=1S/C16H22F8O4/c1-4-10(9(2)3)28-12(26)7-5-6-11(25)27-8-14(19,20)16(23,24)15(21,22)13(17,18)

InchiKey: VHYVUGVPDVZTEK-UHFFFAOYSA-N

Formula: C16H22F8O4

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

Mol. weight [g/mol]: 430.33

Physical Properties

Property code	Value	Unit	Source
gf	-1941.28	kJ/mol	Joback Method
hf	-2474.14	kJ/mol	Joback Method
hfus	34.60	kJ/mol	Joback Method
hvap	57.93	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.849		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1156.14	kPa	Joback Method
rinpol	1623.00		NIST Webbook
rinpol	1623.00		NIST Webbook
tb	701.21	K	Joback Method
tc	864.92	K	Joback Method
tf	381.38	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.90	J/mol×K	701.21	Joback Method
cpg	818.34	J/mol×K	728.50	Joback Method
cpg	831.95	J/mol×K	755.78	Joback Method
cpg	844.75	J/mol×K	783.07	Joback Method
cpg	856.78	J/mol×K	810.35	Joback Method
cpg	868.09	J/mol×K	837.64	Joback Method
cpg	878.71	J/mol×K	864.92	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393491&Units=SI

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