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

Inchi: InChI=1S/C19H20F8O4/c20-16(21)18(24,25)19(26,27)17(22,23)12-31-15(29)10-4-9-14(2

InchiKey: IFMWXBONHNLAKS-UHFFFAOYSA-N

Formula: C19H20F8O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCCCc1ccccc1

Mol. weight [g/mol]: 464.35

Physical Properties

Property code	Value	Unit	Source
gf	-1798.73	kJ/mol	Joback Method
hf	-2288.97	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	67.66	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.047		Crippen Method
mcvol	283.850	ml/mol	McGowan Method
pc	1177.66	kPa	Joback Method
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
tb	797.41	K	Joback Method
tc	980.58	K	Joback Method
tf	471.61	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.78	J/mol×K	797.41	Joback Method
cpg	898.13	J/mol×K	827.94	Joback Method
cpg	910.54	J/mol×K	858.47	Joback Method
cpg	922.06	J/mol×K	888.99	Joback Method
cpg	932.77	J/mol×K	919.52	Joback Method
cpg	942.73	J/mol×K	950.05	Joback Method
cpg	952.01	J/mol×K	980.58	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=U391770&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

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