

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

Inchi: InChI=1S/C19H20F8O5/c1-11(2)31-12-6-3-4-7-13(12)32-15(29)9-5-8-14(28)30-10-17(22)
InchiKey: RVFJRCLGBVIDGD-UHFFFAOYSA-N
Formula: C19H20F8O5
SMILES: CC(C)Oc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]: 480.35

Physical Properties

Property code	Value	Unit	Source
gf	-1915.80	kJ/mol	Joback Method
hf	-2437.94	kJ/mol	Joback Method
hfus	40.73	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.264		Crippen Method
mcvol	289.720	ml/mol	McGowan Method
pc	1158.50	kPa	Joback Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		NIST Webbook
tb	824.37	K	Joback Method
tc	1012.26	K	Joback Method
tf	491.36	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.37	J/molxK	824.37	Joback Method
cpg	925.42	J/molxK	855.69	Joback Method
cpg	937.48	J/molxK	887.00	Joback Method
cpg	948.60	J/molxK	918.32	Joback Method
cpg	958.83	J/molxK	949.63	Joback Method
cpg	968.23	J/molxK	980.95	Joback Method
cpg	976.86	J/molxK	1012.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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