Glutaric acid, 2,2,3,3,4,4,5,5-octafluoropentyl trans-4-tert-butylcyclohexyl ester

Inchi: InChI=1S/C20H28F8O4/c1-17(2,3)12-7-9-13(10-8-12)32-15(30)6-4-5-14(29)31-11-18(23

InchiKey: WJAXMOVDIIRVRJ-UHFFFAOYSA-N

Formula: C20H28F8O4

SMILES: CC(C)(C)C1CCC(OC(=O)CCCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)CC1

Mol. weight [g/mol]: 484.42

Physical Properties

Property code	Value	Unit	Source
gf	-1883.14	kJ/mol	Joback Method
hf	-2520.91	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.019		Crippen Method
mcvol	310.840	ml/mol	McGowan Method
pc	1007.81	kPa	Joback Method
rinpol	2113.00		NIST Webbook
rinpol	2113.00		NIST Webbook
tb	805.26	K	Joback Method
tc	990.03	K	Joback Method
tf	462.02	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.22	J/mol×K	805.26	Joback Method
cpg	1049.92	J/mol×K	836.05	Joback Method
cpg	1065.46	J/mol×K	866.85	Joback Method
cpg	1079.89	J/mol×K	897.64	Joback Method
cpg	1093.30	J/mol×K	928.44	Joback Method
cpg	1105.75	J/mol×K	959.23	Joback Method
cpg	1117.32	J/mol×K	990.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393399&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
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
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