Glutaric acid, 1,1,1-trifluoroprop-2-yl pentafluorobenzyl ester

Inchi: InChI=1S/C15H12F8O4/c1-6(15(21,22)23)27-9(25)4-2-3-8(24)26-5-7-10(16)12(18)14(20)

InchiKey: CQDSUXZTIDSMHS-UHFFFAOYSA-N

Formula: C15H12F8O4

SMILES: CC(OC(=O)CCCC(=O)OCc1c(F)c(F)c(F)c(F)c1F)C(F)(F)F

Mol. weight [g/mol]: 408.24

Physical Properties

Property code	Value	Unit	Source
gf	-1886.24	kJ/mol	Joback Method
hf	-2246.26	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.090		Crippen Method
mcvol	227.490	ml/mol	McGowan Method
pc	1431.55	kPa	Joback Method
rinpol	1632.00		NIST Webbook
rinpol	1632.00		NIST Webbook
tb	737.25	K	Joback Method
tc	910.75	K	Joback Method
tf	484.29	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.22	J/mol×K	737.25	Joback Method
cpg	666.45	J/mol×K	766.17	Joback Method
cpg	677.00	J/mol×K	795.08	Joback Method
cpg	686.87	J/mol×K	824.00	Joback Method
cpg	696.09	J/mol×K	852.92	Joback Method
cpg	704.66	J/mol×K	881.83	Joback Method
cpg	712.59	J/mol×K	910.75	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=U391924&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