Glutaric acid, 2,2,3,3-tetrafluoropropyl 1-phenylpropyl ester

Inchi: InChI=1S/C17H20F4O4/c1-2-13(12-7-4-3-5-8-12)25-15(23)10-6-9-14(22)24-11-17(20,21
InchiKey: PUYFJWCXQFOLOW-UHFFFAOYSA-N
Formula: C17H20F4O4
SMILES: CCC(OC(=O)CCCC(=O)OCC(F)(F)C(F)F)c1ccccc1
Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1044.45	kJ/mol	Joback Method
hf	-1451.03	kJ/mol	Joback Method
hfus	37.26	kJ/mol	Joback Method
hvap	68.68	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.295		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1511.67	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	760.59	K	Joback Method
tc	949.37	K	Joback Method
tf	426.87	K	Joback Method
vc	0.977	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.77	J/mol×K	760.59	Joback Method
cpg	752.89	J/mol×K	792.05	Joback Method
cpg	766.05	J/mol×K	823.52	Joback Method
cpg	778.29	J/mol×K	854.98	Joback Method
cpg	789.63	J/mol×K	886.44	Joback Method
cpg	800.12	J/mol×K	917.90	Joback Method
cpg	809.79	J/mol×K	949.37	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=U392043&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