Glutaric acid, 1,1,1-trifluoroprop-2-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C21H21F3O5/c1-15(21(22,23)24)28-20(26)12-6-11-19(25)27-14-16-7-5-10-18(

InchiKey: ONVBPOIYIXKSPR-UHFFFAOYSA-N

Formula: C21H21F3O5

SMILES: CC(OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1)C(F)(F)F

Mol. weight [g/mol]: 410.38

Physical Properties

Property code	Value	Unit	Source
gf	-815.74	kJ/mol	Joback Method
hf	-1239.36	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	84.14	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.186		Crippen Method
mcvol	285.290	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2477.00		NIST Webbook
tb	907.36	K	Joback Method
tc	1122.83	K	Joback Method
tf	547.53	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	889.50	J/mol×K	907.36	Joback Method
cpg	902.07	J/mol×K	943.27	Joback Method
cpg	913.40	J/mol×K	979.18	Joback Method
cpg	923.51	J/mol×K	1015.09	Joback Method
cpg	932.47	J/mol×K	1051.01	Joback Method
cpg	940.32	J/mol×K	1086.92	Joback Method
cpg	947.11	J/mol×K	1122.83	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=U392119&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