Glutaric acid, 2,2,3,3-tetrafluoropropyl 4-biphenyl ester

Inchi: InChI=1S/C20H18F4O4/c21-19(22)20(23,24)13-27-17(25)7-4-8-18(26)28-16-11-9-15(10-

InchiKey: RXELXZOBYQVGPI-UHFFFAOYSA-N

Formula: C20H18F4O4

SMILES: O=C(CCCC(=O)Oc1ccc(-c2ccccc2)cc1)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 398.35

Physical Properties

Property code	Value	Unit	Source
gf	-913.97	kJ/mol	Joback Method
hf	-1282.61	kJ/mol	Joback Method
hfus	42.21	kJ/mol	Joback Method
hvap	78.69	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.873		Crippen Method
mcvol	267.100	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	861.33	K	Joback Method
tc	1071.29	K	Joback Method
tf	514.62	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.57	J/mol×K	861.33	Joback Method
cpg	825.21	J/mol×K	896.32	Joback Method
cpg	836.75	J/mol×K	931.32	Joback Method
cpg	847.23	J/mol×K	966.31	Joback Method
cpg	856.72	J/mol×K	1001.30	Joback Method
cpg	865.27	J/mol×K	1036.29	Joback Method
cpg	872.94	J/mol×K	1071.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390117&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

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