Glutaric acid, 2,2,3,3-tetrafluoropropyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C21H20F4O5/c22-20(23)21(24,25)14-29-19(27)11-5-10-18(26)28-13-15-6-4-9-

InchiKey: OBOKMVRMDGUVPR-UHFFFAOYSA-N

Formula: C21H20F4O5

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

Mol. weight [g/mol]: 428.37

Physical Properties

Property code	Value	Unit	Source
gf	-1010.55	kJ/mol	Joback Method
hf	-1435.47	kJ/mol	Joback Method
hfus	45.98	kJ/mol	Joback Method
hvap	83.32	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.136		Crippen Method
mcvol	287.060	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		NIST Webbook
tb	906.63	K	Joback Method
tc	1118.17	K	Joback Method
tf	548.12	K	Joback Method
vc	1.117	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.70	J/mol×K	906.63	Joback Method
cpg	908.93	J/mol×K	941.89	Joback Method
cpg	919.95	J/mol×K	977.14	Joback Method
cpg	929.81	J/mol×K	1012.40	Joback Method
cpg	938.56	J/mol×K	1047.66	Joback Method
cpg	946.23	J/mol×K	1082.91	Joback Method
cpg	952.88	J/mol×K	1118.17	Joback Method

Sources

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=U392120&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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