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

Inchi: InChI=1S/C17H20F4O4/c18-16(19)17(20,21)12-25-15(23)10-4-9-14(22)24-11-5-8-13-6-2

InchiKey: DVFQAOKJFYOLNL-UHFFFAOYSA-N

Formula: C17H20F4O4

SMILES: O=C(CCCC(=O)OCC(F)(F)C(F)F)OCCCc1ccccc1

Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1042.01	kJ/mol	Joback Method
hf	-1445.75	kJ/mol	Joback Method
hfus	40.78	kJ/mol	Joback Method
hvap	69.07	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.776		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook
tb	761.03	K	Joback Method
tc	947.82	K	Joback Method
tf	441.87	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	738.23	J/mol×K	761.03	Joback Method
cpg	752.19	J/mol×K	792.16	Joback Method
cpg	765.22	J/mol×K	823.29	Joback Method
cpg	777.35	J/mol×K	854.42	Joback Method
cpg	788.62	J/mol×K	885.55	Joback Method
cpg	799.06	J/mol×K	916.69	Joback Method
cpg	808.71	J/mol×K	947.82	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=U391769&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