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

Inchi: InChI=1S/C17H20F4O4/c1-2-6-12-7-3-4-8-13(12)25-15(23)10-5-9-14(22)24-11-17(20,21
InchiKey: KLRUCHLGUTUIEU-UHFFFAOYSA-N
Formula: C17H20F4O4
SMILES: CCCc1ccccc1OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1051.64	kJ/mol	Joback Method
hf	-1457.22	kJ/mol	Joback Method
hfus	40.39	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.158		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	1938.00		NIST Webbook
rinpol	1938.00		NIST Webbook
tb	766.01	K	Joback Method
tc	953.66	K	Joback Method
tf	454.39	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.41	J/mol×K	766.01	Joback Method
cpg	751.27	J/mol×K	797.28	Joback Method
cpg	764.21	J/mol×K	828.56	Joback Method
cpg	776.26	J/mol×K	859.83	Joback Method
cpg	787.45	J/mol×K	891.11	Joback Method
cpg	797.82	J/mol×K	922.38	Joback Method
cpg	807.38	J/mol×K	953.66	Joback Method

Sources

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=U392135&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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