Glutaric acid, pentyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C17H21F3O4/c1-2-3-4-10-23-15(21)6-5-7-16(22)24-11-12-13(18)8-9-14(19)17
InchiKey: YNKQOUGZDWIVIR-UHFFFAOYSA-N
Formula: C17H21F3O4
SMILES: CCCCCOC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F
Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-876.49	kJ/mol	Joback Method
hf	-1270.02	kJ/mol	Joback Method
hfus	47.47	kJ/mol	Joback Method
hvap	73.56	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.051		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1471.36	kPa	Joback Method
rinpol	2146.00		NIST Webbook
rinpol	2146.00		NIST Webbook
tb	780.37	K	Joback Method
tc	967.40	K	Joback Method
tf	491.42	K	Joback Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.65	J/mol×K	780.37	Joback Method
cpg	739.50	J/mol×K	811.54	Joback Method
cpg	752.48	J/mol×K	842.71	Joback Method
cpg	764.60	J/mol×K	873.89	Joback Method
cpg	775.87	J/mol×K	905.06	Joback Method
cpg	786.29	J/mol×K	936.23	Joback Method
cpg	795.86	J/mol×K	967.40	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=U376897&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