Glutaric acid, isobutyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C17H21F3O5/c1-12(2)10-23-15(21)4-3-5-16(22)24-11-13-6-8-14(9-7-13)25-17

InchiKey: IWJUQSSDYDCOAX-UHFFFAOYSA-N

Formula: C17H21F3O5

SMILES: CC(C)COC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 362.34

Physical Properties

Property code	Value	Unit	Source
gf	-961.83	kJ/mol	Joback Method
hf	-1393.33	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	72.96	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.998		Crippen Method
mcvol	252.690	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2036.00		NIST Webbook
tb	789.16	K	Joback Method
tc	982.22	K	Joback Method
tf	476.03	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.65	J/mol×K	789.16	Joback Method
cpg	771.60	J/mol×K	821.34	Joback Method
cpg	784.56	J/mol×K	853.51	Joback Method
cpg	796.55	J/mol×K	885.69	Joback Method
cpg	807.58	J/mol×K	917.87	Joback Method
cpg	817.69	J/mol×K	950.05	Joback Method
cpg	826.87	J/mol×K	982.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377335&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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