Glutaric acid, ethyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C15H17F3O5/c1-2-21-13(19)4-3-5-14(20)22-10-11-6-8-12(9-7-11)23-15(16,17

InchiKey: UVUZVVVQXNVHIQ-UHFFFAOYSA-N

Formula: C15H17F3O5

SMILES: CCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1

Mol. weight [g/mol]: 334.29

Physical Properties

Property code	Value	Unit	Source
gf	-976.23	kJ/mol	Joback Method
hf	-1346.77	kJ/mol	Joback Method
hfus	36.85	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.362		Crippen Method
mcvol	224.510	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpol	1881.00		NIST Webbook
rinpol	1881.00		NIST Webbook
tb	743.84	K	Joback Method
tc	935.11	K	Joback Method
tf	468.49	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.43	J/mol×K	743.84	Joback Method
cpg	659.56	J/mol×K	775.72	Joback Method
cpg	671.82	J/mol×K	807.60	Joback Method
cpg	683.20	J/mol×K	839.47	Joback Method
cpg	693.73	J/mol×K	871.35	Joback Method
cpg	703.42	J/mol×K	903.23	Joback Method
cpg	712.29	J/mol×K	935.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377333&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