Glutaric acid, ethyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C15H17F3O4/c1-2-21-13(19)4-3-5-14(20)22-10-11-6-8-12(9-7-11)15(16,17)18

InchiKey: TZUBCNITOKPPEG-UHFFFAOYSA-N

Formula: C15H17F3O4

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

Mol. weight [g/mol]: 318.29

Physical Properties

Property code	Value	Unit	Source
gf	-871.23	kJ/mol	Joback Method
hf	-1214.55	kJ/mol	Joback Method
hfus	35.66	kJ/mol	Joback Method
hvap	66.49	kJ/mol	Joback Method
log10ws	-4.11		Crippen Method
logp	3.482		Crippen Method
mcvol	218.640	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
rinpol	1997.00		NIST Webbook
tb	721.42	K	Joback Method
tc	912.88	K	Joback Method
tf	446.26	K	Joback Method
vc	0.859	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.55	J/mol×K	721.42	Joback Method
cpg	632.98	J/mol×K	753.33	Joback Method
cpg	645.53	J/mol×K	785.24	Joback Method
cpg	657.25	J/mol×K	817.15	Joback Method
cpg	668.14	J/mol×K	849.06	Joback Method
cpg	678.24	J/mol×K	880.97	Joback Method
cpg	687.57	J/mol×K	912.88	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=U377576&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