

Glutaric acid, isobutyl 4-(trifluoromethyl)benzyl ester

Inchi:	InChI=1S/C17H21F3O4/c1-12(2)10-23-15(21)4-3-5-16(22)24-11-13-6-8-14(9-7-13)17(18)
InchiKey:	WISDHGZRSQMLAJ-UHFFFAOYSA-N
Formula:	C17H21F3O4
SMILES:	CC(C)COC(=O)CCCC(=O)OCc1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]:	346.34

Physical Properties

Property code	Value	Unit	Source
gf	-856.83	kJ/mol	Joback Method
hf	-1261.11	kJ/mol	Joback Method
hfus	37.31	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.118		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1537.87	kPa	Joback Method
rinqol	2165.00		NIST Webbook
tb	766.74	K	Joback Method
tc	959.29	K	Joback Method
tf	453.80	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.74	J/molxK	766.74	Joback Method
cpg	744.04	J/molxK	798.83	Joback Method
cpg	757.38	J/molxK	830.92	Joback Method
cpg	769.80	J/molxK	863.02	Joback Method
cpg	781.31	J/molxK	895.11	Joback Method
cpg	791.96	J/molxK	927.20	Joback Method
cpg	801.78	J/molxK	959.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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

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