

Glutaric acid, butyl 4-(trifluoromethoxy)benzyl ester

Inchi:	InChI=1S/C17H21F3O5/c1-2-3-11-23-15(21)5-4-6-16(22)24-12-13-7-9-14(10-8-13)25-17
InchiKey:	DKMDXPOWUILCRO-UHFFFAOYSA-N
Formula:	C17H21F3O5
SMILES:	CCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]:	362.34

Physical Properties

Property code	Value	Unit	Source
gf	-959.39	kJ/mol	Joback Method
hf	-1388.05	kJ/mol	Joback Method
hfus	42.03	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.142		Crippen Method
mvol	252.690	ml/mol	McGowan Method
pc	1508.15	kPa	Joback Method
rinpol	2079.00		NIST Webbook
rinpol	2079.00		NIST Webbook
tb	789.60	K	Joback Method
tc	980.78	K	Joback Method
tf	491.03	K	Joback Method
vc	0.989	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.10	J/mol×K	789.60	Joback Method
cpg	770.91	J/mol×K	821.46	Joback Method
cpg	783.76	J/mol×K	853.33	Joback Method
cpg	795.66	J/mol×K	885.19	Joback Method
cpg	806.64	J/mol×K	917.05	Joback Method
cpg	816.72	J/mol×K	948.91	Joback Method
cpg	825.91	J/mol×K	980.78	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=U377336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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