

Glutaric acid, butyl 2,3,4,5-tetrafluorobenzyl ester

Inchi:	InChI=1S/C16H18F4O4/c1-2-3-7-23-12(21)5-4-6-13(22)24-9-10-8-11(17)15(19)16(20)14
InchiKey:	MYOXPXZPGKFOHF-UHFFFAOYSA-N
Formula:	C16H18F4O4
SMILES:	CCCCOC(=O)CCCC(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]:	350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1089.35	kJ/mol	Joback Method
hf	-1456.96	kJ/mol	Joback Method
hfus	47.57	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.800		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1512.85	kPa	Joback Method
rinpola	2034.00		NIST Webbook
rinpola	2034.00		NIST Webbook
tb	761.74	K	Joback Method
tc	944.71	K	Joback Method
tf	493.26	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.72	J/molxK	761.74	Joback Method
cpg	689.69	J/molxK	792.24	Joback Method
cpg	701.88	J/molxK	822.73	Joback Method
cpg	713.30	J/molxK	853.23	Joback Method
cpg	723.94	J/molxK	883.72	Joback Method
cpg	733.81	J/molxK	914.22	Joback Method
cpg	742.90	J/molxK	944.71	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=U377441&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
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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