Glutaric acid, isobutyl 2,3,6-trifluorobenzyl ester

Inchi: InChI=1S/C16H19F3O4/c1-10(2)8-22-14(20)4-3-5-15(21)23-9-11-12(17)6-7-13(18)16(11

InchiKey: UAAGQZDKILSUGC-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: CC(C)COC(=O)CCCC(=O)OCc1c(F)ccc(F)c1F

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-887.35	kJ/mol	Joback Method
hf	-1254.66	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	70.94	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.517		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	2002.00		NIST Webbook
tb	757.05	K	Joback Method
tc	945.48	K	Joback Method
tf	465.15	K	Joback Method
vc	0.919	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.48	J/mol×K	757.05	Joback Method
cpg	684.07	J/mol×K	788.46	Joback Method
cpg	696.82	J/mol×K	819.86	Joback Method
cpg	708.74	J/mol×K	851.27	Joback Method
cpg	719.82	J/mol×K	882.67	Joback Method
cpg	730.08	J/mol×K	914.08	Joback Method
cpg	739.51	J/mol×K	945.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376895&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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