Glutaric acid, 2-fluoro-6-(trifluoromethyl)benzyl propyl ester

Inchi: InChI=1S/C16H18F4O4/c1-2-9-23-14(21)7-4-8-15(22)24-10-11-12(16(18,19)20)5-3-6-13

InchiKey: MOVNVRWCKFTSSI-UHFFFAOYSA-N

Formula: C16H18F4O4

SMILES: CCCOC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 350.31

Physical Properties

Property code	Value	Unit	Source
gf	-1067.25	kJ/mol	Joback Method
hf	-1442.77	kJ/mol	Joback Method
hfus	40.94	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.011		Crippen Method
mcvol	234.500	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	748.55	K	Joback Method
tc	934.84	K	Joback Method
tf	470.64	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.70	J/mol×K	748.55	Joback Method
cpg	693.94	J/mol×K	779.60	Joback Method
cpg	706.34	J/mol×K	810.65	Joback Method
cpg	717.91	J/mol×K	841.69	Joback Method
cpg	728.69	J/mol×K	872.74	Joback Method
cpg	738.69	J/mol×K	903.79	Joback Method
cpg	747.93	J/mol×K	934.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377497&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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