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

Inchi: InChI=1S/C17H20F4O4/c1-11(2)9-24-15(22)7-4-8-16(23)25-10-12-13(17(19,20)21)5-3-6
InchiKey: OLQOMDAVMOUSTQ-UHFFFAOYSA-N
Formula: C17H20F4O4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1c(F)cccc1C(F)(F)F
Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1061.27	kJ/mol	Joback Method
hf	-1468.69	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	70.40	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.257		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	770.99	K	Joback Method
tc	959.50	K	Joback Method
tf	466.91	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.56	J/mol×K	770.99	Joback Method
cpg	750.32	J/mol×K	802.41	Joback Method
cpg	763.18	J/mol×K	833.83	Joback Method
cpg	775.15	J/mol×K	865.24	Joback Method
cpg	786.27	J/mol×K	896.66	Joback Method
cpg	796.55	J/mol×K	928.08	Joback Method
cpg	806.03	J/mol×K	959.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377498&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