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

Inchi: InChI=1S/C23H32F4O4/c1-2-3-4-5-6-7-8-9-16-30-21(28)14-11-15-22(29)31-17-18-19(23

InchiKey: SQCLGQBKPRJBMT-UHFFFAOYSA-N

Formula: C23H32F4O4

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

Mol. weight [g/mol]: 448.49

Physical Properties

Property code	Value	Unit	Source
gf	-1008.31	kJ/mol	Joback Method
hf	-1587.25	kJ/mol	Joback Method
hfus	59.07	kJ/mol	Joback Method
hvap	84.14	kJ/mol	Joback Method
log10ws	-7.79		Crippen Method
logp	6.742		Crippen Method
mcvol	333.130	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	2858.00		NIST Webbook
rinpol	2858.00		NIST Webbook
tb	908.71	K	Joback Method
tc	1112.56	K	Joback Method
tf	549.53	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1086.19	J/mol×K	908.71	Joback Method
cpg	1102.05	J/mol×K	942.68	Joback Method
cpg	1116.71	J/mol×K	976.66	Joback Method
cpg	1130.21	J/mol×K	1010.63	Joback Method
cpg	1142.59	J/mol×K	1044.61	Joback Method
cpg	1153.91	J/mol×K	1078.58	Joback Method
cpg	1164.21	J/mol×K	1112.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377506&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

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