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

Inchi: InChI=1S/C21H28F4O4/c1-2-3-4-5-6-7-14-28-19(26)12-9-13-20(27)29-15-16-17(21(23,2

InchiKey: NTPZJKNEPCALRL-UHFFFAOYSA-N

Formula: C21H28F4O4

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

Mol. weight [g/mol]: 420.44

Physical Properties

Property code	Value	Unit	Source
gf	-1025.15	kJ/mol	Joback Method
hf	-1545.97	kJ/mol	Joback Method
hfus	53.89	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.962		Crippen Method
mcvol	304.950	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpol	2634.00		NIST Webbook
tb	862.95	K	Joback Method
tc	1057.84	K	Joback Method
tf	526.99	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.41	J/mol×K	862.95	Joback Method
cpg	981.49	J/mol×K	895.43	Joback Method
cpg	995.49	J/mol×K	927.91	Joback Method
cpg	1008.46	J/mol×K	960.40	Joback Method
cpg	1020.43	J/mol×K	992.88	Joback Method
cpg	1031.44	J/mol×K	1025.36	Joback Method
cpg	1041.53	J/mol×K	1057.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377504&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