Glutaric acid, decyl 4-(trifluoromethyl)benzyl ester

Inchi: InChI=1S/C23H33F3O4/c1-2-3-4-5-6-7-8-9-17-29-21(27)11-10-12-22(28)30-18-19-13-15

InchiKey: PXAWAMVOMWYIFP-UHFFFAOYSA-N

Formula: C23H33F3O4

SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 430.50

Physical Properties

Property code	Value	Unit	Source
gf	-803.87	kJ/mol	Joback Method
hf	-1379.67	kJ/mol	Joback Method
hfus	56.38	kJ/mol	Joback Method
hvap	84.30	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.603		Crippen Method
mcvol	331.360	ml/mol	McGowan Method
pc	1018.13	kPa	Joback Method
rinpol	2853.00		NIST Webbook
rinpol	2853.00		NIST Webbook
tb	904.46	K	Joback Method
tc	1107.50	K	Joback Method
tf	536.42	K	Joback Method
vc	1.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1079.73	J/mol×K	904.46	Joback Method
cpg	1095.80	J/mol×K	938.30	Joback Method
cpg	1110.68	J/mol×K	972.14	Joback Method
cpg	1124.42	J/mol×K	1005.98	Joback Method
cpg	1137.06	J/mol×K	1039.82	Joback Method
cpg	1148.67	J/mol×K	1073.66	Joback Method
cpg	1159.29	J/mol×K	1107.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377585&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