Glutaric acid, decyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C23H33F3O5/c1-2-3-4-5-6-7-8-9-17-29-21(27)11-10-12-22(28)30-18-19-13-15

InchiKey: FZQITBSABYMTJU-UHFFFAOYSA-N

Formula: C23H33F3O5

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

Mol. weight [g/mol]: 446.50

Physical Properties

Property code	Value	Unit	Source
gf	-908.87	kJ/mol	Joback Method
hf	-1511.89	kJ/mol	Joback Method
hfus	57.57	kJ/mol	Joback Method
hvap	86.70	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.483		Crippen Method
mcvol	337.230	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2672.00		NIST Webbook
rinpol	2672.00		NIST Webbook
tb	926.88	K	Joback Method
tc	1134.80	K	Joback Method
tf	558.65	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1109.16	J/mol×K	926.88	Joback Method
cpg	1124.78	J/mol×K	961.53	Joback Method
cpg	1139.08	J/mol×K	996.19	Joback Method
cpg	1152.09	J/mol×K	1030.84	Joback Method
cpg	1163.85	J/mol×K	1065.49	Joback Method
cpg	1174.41	J/mol×K	1100.14	Joback Method
cpg	1183.81	J/mol×K	1134.80	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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