Glutaric acid, dodecyl 4-(trifluoromethoxy)benzyl ester

Inchi: InChI=1S/C25H37F3O5/c1-2-3-4-5-6-7-8-9-10-11-19-31-23(29)13-12-14-24(30)32-20-21
InchiKey: UFNKBBBTQLSLFS-UHFFFAOYSA-N
Formula: C25H37F3O5
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 474.55

Physical Properties

Property code	Value	Unit	Source
gf	-892.03	kJ/mol	Joback Method
hf	-1553.17	kJ/mol	Joback Method
hfus	62.75	kJ/mol	Joback Method
hvap	91.16	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.263		Crippen Method
mcvol	365.410	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	2876.00		NIST Webbook
rinpol	2876.00		NIST Webbook
tb	972.64	K	Joback Method
tc	1193.47	K	Joback Method
tf	581.19	K	Joback Method
vc	1.437	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1231.46	J/mol×K	972.64	Joback Method
cpg	1247.80	J/mol×K	1009.45	Joback Method
cpg	1262.60	J/mol×K	1046.25	Joback Method
cpg	1275.92	J/mol×K	1083.06	Joback Method
cpg	1287.83	J/mol×K	1119.86	Joback Method
cpg	1298.38	J/mol×K	1156.67	Joback Method
cpg	1307.62	J/mol×K	1193.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377343&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