Glutaric acid, 2,5-difluorobenzyl dodecyl ester

Inchi: InChI=1S/C24H36F2O4/c1-2-3-4-5-6-7-8-9-10-11-17-29-23(27)13-12-14-24(28)30-19-20
InchiKey: OOSZUFXZGZHESZ-UHFFFAOYSA-N
Formula: C24H36F2O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 426.54

Physical Properties

Property code	Value	Unit	Source
gf	-613.11	kJ/mol	Joback Method
hf	-1206.92	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	89.30	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.642		Crippen Method
mcvol	343.680	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2852.00		NIST Webbook
rinpol	2852.00		NIST Webbook
tb	936.28	K	Joback Method
tc	1146.56	K	Joback Method
tf	557.20	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1132.84	J/mol×K	936.28	Joback Method
cpg	1149.49	J/mol×K	971.33	Joback Method
cpg	1164.76	J/mol×K	1006.37	Joback Method
cpg	1178.68	J/mol×K	1041.42	Joback Method
cpg	1191.29	J/mol×K	1076.47	Joback Method
cpg	1202.62	J/mol×K	1111.51	Joback Method
cpg	1212.71	J/mol×K	1146.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376954&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