Glutaric acid, 3-fluorobenzyl tridecyl ester

Inchi: InChI=1S/C25H39FO4/c1-2-3-4-5-6-7-8-9-10-11-12-19-29-24(27)17-14-18-25(28)30-21-2
InchiKey: XQORPCDSMFACAN-UHFFFAOYSA-N
Formula: C25H39FO4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(F)c1
Mol. weight [g/mol]: 422.57

Physical Properties

Property code	Value	Unit	Source
gf	-400.25	kJ/mol	Joback Method
hf	-1019.98	kJ/mol	Joback Method
hfus	62.81	kJ/mol	Joback Method
hvap	91.68	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.893		Crippen Method
mcvol	356.000	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	954.91	K	Joback Method
tc	1169.45	K	Joback Method
tf	555.36	K	Joback Method
vc	1.393	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1188.22	J/mol×K	954.91	Joback Method
cpg	1205.40	J/mol×K	990.67	Joback Method
cpg	1221.13	J/mol×K	1026.42	Joback Method
cpg	1235.46	J/mol×K	1062.18	Joback Method
cpg	1248.43	J/mol×K	1097.94	Joback Method
cpg	1260.08	J/mol×K	1133.69	Joback Method
cpg	1270.46	J/mol×K	1169.45	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376975&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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