

Glutaric acid, 3-fluorophenyl octadecyl ester

Inchi: InChI=1S/C29H47FO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-24-33-28(31)22-19-20
InchiKey: AWEMROCYQXFIAN-UHFFFAOYSA-N
Formula: C29H47FO4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 478.68

Physical Properties

Property code	Value	Unit	Source
gf	-366.57	kJ/mol	Joback Method
hf	-1102.54	kJ/mol	Joback Method
hfus	73.17	kJ/mol	Joback Method
hvap	100.58	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.706		Crippen Method
mvol	412.360	ml/mol	McGowan Method
pc	755.15	kPa	Joback Method
rinpol	3451.00		NIST Webbook
rinpol	3451.00		NIST Webbook
tb	1046.43	K	Joback Method
tc	1294.45	K	Joback Method
tf	600.44	K	Joback Method
vc	1.617	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1439.60	J/molxK	1046.43	Joback Method
cpg	1458.39	J/molxK	1087.77	Joback Method
cpg	1475.19	J/molxK	1129.10	Joback Method
cpg	1490.09	J/molxK	1170.44	Joback Method
cpg	1503.19	J/molxK	1211.78	Joback Method
cpg	1514.56	J/molxK	1253.11	Joback Method
cpg	1524.31	J/molxK	1294.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359062&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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