

Glutaric acid, 1-(4-fluorophenyl)ethyl undecyl ester

Inchi:	InChI=1S/C24H37FO4/c1-3-4-5-6-7-8-9-10-11-19-28-23(26)13-12-14-24(27)29-20(2)21-
InchiKey:	FPFONFYAWYLLCP-UHFFFAOYSA-N
Formula:	C24H37FO4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OC(C)c1ccc(F)cc1
Mol. weight [g/mol]:	408.55

Physical Properties

Property code	Value	Unit	Source
gf	-411.11	kJ/mol	Joback Method
hf	-1004.62	kJ/mol	Joback Method
hfus	56.70	kJ/mol	Joback Method
hvap	89.06	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	6.674		Crippen Method
mvol	341.910	ml/mol	McGowan Method
pc	1007.17	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	931.59	K	Joback Method
tc	1140.67	K	Joback Method
tf	529.09	K	Joback Method
vc	1.331	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.85	J/molxK	931.59	Joback Method
cpg	1143.68	J/molxK	966.44	Joback Method
cpg	1159.14	J/molxK	1001.28	Joback Method
cpg	1173.26	J/molxK	1036.13	Joback Method
cpg	1186.10	J/molxK	1070.98	Joback Method
cpg	1197.67	J/molxK	1105.82	Joback Method
cpg	1208.04	J/molxK	1140.67	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=U377109&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/95-535-3/Glutaric-acid-1-4-fluorophenyl-ethyl-undecyl-ester.pdf>

Generated by Cheméo on 2024-04-19 19:48:58.405877506 +0000 UTC m=+15845387.326454821.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.