Glutaric acid, 2-(2-fluorophenyl)ethyl heptyl ester

Inchi: InChI=1S/C20H29FO4/c1-2-3-4-5-8-15-24-19(22)12-9-13-20(23)25-16-14-17-10-6-7-11-1

InchiKey: PVKLYFLJWIDCGS-UHFFFAOYSA-N

Formula: C20H29FO4

SMILES: CCCCCCCOC(=O)CCCC(=O)OCCc1ccccc1F

Mol. weight [g/mol]: 352.44

Physical Properties

Property code	Value	Unit	Source
gf	-442.35	kJ/mol	Joback Method
hf	-916.78	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.595		Crippen Method
mcvol	285.550	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2485.00		NIST Webbook
rinpol	2485.00		NIST Webbook
tb	840.51	K	Joback Method
tc	1036.82	K	Joback Method
tf	499.01	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.09	J/mol×K	840.51	Joback Method
cpg	900.82	J/mol×K	873.23	Joback Method
cpg	915.47	J/mol×K	905.95	Joback Method
cpg	929.04	J/mol×K	938.67	Joback Method
cpg	941.57	J/mol×K	971.38	Joback Method
cpg	953.08	J/mol×K	1004.10	Joback Method
cpg	963.58	J/mol×K	1036.82	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377088&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
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
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