Glutaric acid, 2-(adamant-1-yl)ethyl 2-fluorophenyl ester

Inchi: InChI=1S/C23H29FO4/c24-19-4-1-2-5-20(19)28-22(26)7-3-6-21(25)27-9-8-23-13-16-10-1

InchiKey: TUMCXIZUMPVPFL-UHFFFAOYSA-N

Formula: C23H29FO4

SMILES: O=C(CCCC(=O)Oc1ccccc1F)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 388.47

Physical Properties

Property code	Value	Unit	Source
gf	-260.14	kJ/mol	Joback Method
hf	-771.56	kJ/mol	Joback Method
hfus	44.71	kJ/mol	Joback Method
hvap	85.68	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.051		Crippen Method
mcvol	295.240	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
rinpol	2984.00		NIST Webbook
rinpol	2984.00		NIST Webbook
tb	929.21	K	Joback Method
tc	1153.21	K	Joback Method
tf	602.78	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1022.62	J/mol×K	929.21	Joback Method
cpg	1043.19	J/mol×K	966.54	Joback Method
cpg	1063.56	J/mol×K	1003.88	Joback Method
cpg	1083.94	J/mol×K	1041.21	Joback Method
cpg	1104.55	J/mol×K	1078.54	Joback Method
cpg	1125.59	J/mol×K	1115.88	Joback Method
cpg	1147.28	J/mol×K	1153.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405383&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