Glutaric acid, naphth-2-ylmethyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C22H18ClFO4/c23-18-7-3-8-19(24)22(18)28-21(26)10-4-9-20(25)27-14-15-11-

InchiKey: MIRLMDWNUSBMFI-UHFFFAOYSA-N

Formula: C22H18ClFO4

SMILES: O=C(CCCC(=O)Oc1c(F)cccc1Cl)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 400.83

Physical Properties

Property code	Value	Unit	Source
gf	-237.64	kJ/mol	Joback Method
hf	-569.14	kJ/mol	Joback Method
hfus	49.52	kJ/mol	Joback Method
hvap	94.62	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.451		Crippen Method
mcvol	282.750	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook
tb	979.32	K	Joback Method
tc	1216.30	K	Joback Method
tf	635.63	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.85	J/mol×K	979.32	Joback Method
cpg	852.86	J/mol×K	1018.82	Joback Method
cpg	862.76	J/mol×K	1058.31	Joback Method
cpg	871.64	J/mol×K	1097.81	Joback Method
cpg	879.57	J/mol×K	1137.31	Joback Method
cpg	886.61	J/mol×K	1176.80	Joback Method
cpg	892.84	J/mol×K	1216.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391592&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