

Glutaric acid, 2-chloro-6-fluorophenyl 1-naphthyl ester

Inchi:	InChI=1S/C21H16ClFO4/c22-16-9-4-10-17(23)21(16)27-20(25)13-5-12-19(24)26-18-11-3
InchiKey:	GCQQGTKIJDEJCS-UHFFFAOYSA-N
Formula:	C21H16ClFO4
SMILES:	O=C(CCCC(=O)Oc1cccc2ccccc12)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	386.80

Physical Properties

Property code	Value	Unit	Source
gf	-246.06	kJ/mol	Joback Method
hf	-548.50	kJ/mol	Joback Method
hfus	46.93	kJ/mol	Joback Method
hvap	92.40	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.314		Crippen Method
mvol	268.660	ml/mol	McGowan Method
pc	1792.42	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	956.44	K	Joback Method
tc	1194.46	K	Joback Method
tf	624.36	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.34	J/molxK	956.44	Joback Method
cpg	795.16	J/molxK	996.11	Joback Method
cpg	804.89	J/molxK	1035.78	Joback Method
cpg	813.60	J/molxK	1075.45	Joback Method
cpg	821.35	J/molxK	1115.12	Joback Method
cpg	828.21	J/molxK	1154.79	Joback Method
cpg	834.26	J/molxK	1194.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390319&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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