

Glutaric acid, 2-chloro-6-fluorophenyl nonyl ester

Inchi:	InChI=1S/C20H28ClFO4/c1-2-3-4-5-6-7-8-15-25-18(23)13-10-14-19(24)26-20-16(21)11-9
InchiKey:	FJWBCKWBOCCYMK-UHFFFAOYSA-N
Formula:	C20H28ClFO4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)Oc1c(F)cccc1Cl
Mol. weight [g/mol]:	386.88

Physical Properties

Property code	Value	Unit	Source
gf	-463.91	kJ/mol	Joback Method
hf	-943.99	kJ/mol	Joback Method
hfus	53.67	kJ/mol	Joback Method
hvap	85.59	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.849		Crippen Method
mvol	297.790	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2619.00		NIST Webbook
rinpol	2619.00		NIST Webbook
tb	882.92	K	Joback Method
tc	1086.02	K	Joback Method
tf	541.45	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.35	J/mol×K	882.92	Joback Method
cpg	925.90	J/mol×K	916.77	Joback Method
cpg	939.32	J/mol×K	950.62	Joback Method
cpg	951.64	J/mol×K	984.47	Joback Method
cpg	962.86	J/mol×K	1018.32	Joback Method
cpg	973.02	J/mol×K	1052.17	Joback Method
cpg	982.14	J/mol×K	1086.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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