

Glutaric acid, 2,4,6-trichlorophenyl 3-fluorophenyl ester

Inchi:	InChI=1S/C17H12Cl3FO4/c18-10-7-13(19)17(14(20)8-10)25-16(23)6-2-5-15(22)24-12-4
InchiKey:	XUURGMLMNVUKDE-UHFFFAOYSA-N
Formula:	C17H12Cl3FO4
SMILES:	O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1cccc(F)c1
Mol. weight [g/mol]:	405.63

Physical Properties

Property code	Value	Unit	Source
gf	-419.88	kJ/mol	Joback Method
hf	-699.96	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.467		Crippen Method
mcvol	256.240	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpola	2750.00		NIST Webbook
rinpola	2750.00		NIST Webbook
tb	925.78	K	Joback Method
tc	1160.71	K	Joback Method
tf	618.94	K	Joback Method
vc	0.985	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.05	J/molxK	925.78	Joback Method
cpg	687.03	J/molxK	964.94	Joback Method
cpg	694.85	J/molxK	1004.09	Joback Method
cpg	701.53	J/molxK	1043.25	Joback Method
cpg	707.10	J/molxK	1082.40	Joback Method
cpg	711.56	J/molxK	1121.56	Joback Method
cpg	714.94	J/molxK	1160.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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