

Fluoroglycofen ethyl ester

Other names:	Benzoic acid, 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitro-, ester with ethyl glycolate BAS 9106 H Benzoic acid, 5-(2-chloro-4-(trifluoromethyl)phenoxy)-2-nitro-, 2-ethoxy-2-oxoethyl ester Fluoroglycofen Fluoroglycofen-ethyl RH-0265 Super blazer
Inchi:	InChI=1S/C18H13ClF3NO7/c1-2-28-16(24)9-29-17(25)12-8-11(4-5-14(12)23(26)27)30-1
InchiKey:	IPPAUTOBDWNLX-UHFFFAOYSA-N
Formula:	C18H13ClF3NO7
SMILES:	CCOC(=O)COC(=O)c1cc(Oc2ccc(C(F)(F)F)cc2Cl)ccc1[N+](=O)[O-]
Mol. weight [g/mol]:	447.75
CAS:	77501-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-843.83	kJ/mol	Joback Method
hf	-1233.07	kJ/mol	Joback Method
hfus	53.05	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.779		Crippen Method
mvol	272.680	ml/mol	McGowan Method
pc	1721.73	kPa	Joback Method
tb	1043.37	K	Joback Method
tc	1286.24	K	Joback Method
tf	739.81	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.77	J/mol×K	1043.37	Joback Method
cpg	824.10	J/mol×K	1083.85	Joback Method

cpg	829.09	J/mol×K	1124.33	Joback Method
cpg	832.77	J/mol×K	1164.80	Joback Method
cpg	835.19	J/mol×K	1205.28	Joback Method
cpg	836.38	J/mol×K	1245.76	Joback Method
cpg	836.37	J/mol×K	1286.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77501907&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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