

Diflunisal di-methyl derivative

Other names:

Diflunisal, bis-methylated
Diflunisal, methyl ether, methyl ester
Diflusinal Me
Diflunisal, methylated

Inchi:

InChI=1S/C15H12F2O3/c1-19-14-6-3-9(7-12(14)15(18)20-2)11-5-4-10(16)8-13(11)17/h3

InchiKey:

JIZOQURFDNMVQH-UHFFFAOYSA-N

Formula:

C15H12F2O3

SMILES:

COC(=O)c1cc(-c2ccc(F)cc2F)ccc1OC

Mol. weight [g/mol]:

278.25

CAS:

268746-73-2

Physical Properties

Property code	Value	Unit	Source
gf	-466.82	kJ/mol	Joback Method
hf	-694.99	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	66.12	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	3.427		Crippen Method
mcvol	191.540	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
tb	713.13	K	Joback Method
tc	931.03	K	Joback Method
tf	457.30	K	Joback Method
vc	0.738	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.17	J/molxK	713.13	Joback Method
cpg	517.49	J/molxK	749.45	Joback Method
cpg	529.87	J/molxK	785.76	Joback Method

cpg	541.33	J/mol×K	822.08	Joback Method
cpg	551.86	J/mol×K	858.40	Joback Method
cpg	561.47	J/mol×K	894.72	Joback Method
cpg	570.16	J/mol×K	931.03	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C268746732&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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