

Diphenacyl isophthalate

Inchi:

lnchl=1S/C24H18O6/c25-21(17-8-3-1-4-9-17)15-29-23(27)19-12-7-13-20(14-19)24(28)3

InchiKey:

NWTODHNVXLOHFQ-UHFFFAOYSA-N

Formula:

C24H18O6

SMILES:

O=C(COC(=O)c1cccc(C(=O)OCC(=O)c2ccccc2)c1)c1ccccc1

Mol. weight [g/mol]:

402.40

CAS:

116345-97-2

Physical Properties

Property code	Value	Unit	Source
gf	-246.88	kJ/mol	Joback Method
hf	-555.33	kJ/mol	Joback Method
hfus	48.42	kJ/mol	Joback Method
hvap	108.31	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	3.766		Crippen Method
mcvol	295.760	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
tb	1093.86	K	Joback Method
tc	1351.75	K	Joback Method
tf	696.20	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	913.01	J/mol×K	1093.86	Joback Method
cpg	920.13	J/mol×K	1136.84	Joback Method
cpg	925.77	J/mol×K	1179.82	Joback Method
cpg	930.04	J/mol×K	1222.80	Joback Method
cpg	933.01	J/mol×K	1265.78	Joback Method
cpg	934.77	J/mol×K	1308.77	Joback Method
cpg	935.41	J/mol×K	1351.75	Joback Method
dvisc	0.0002189	Pa×s	696.20	Joback Method
dvisc	0.0001354	Pa×s	762.48	Joback Method

dvisc	0.0000904	Pa×s	828.75	Joback Method
dvisc	0.0000641	Pa×s	895.03	Joback Method
dvisc	0.0000477	Pa×s	961.31	Joback Method
dvisc	0.0000368	Pa×s	1027.58	Joback Method
dvisc	0.0000293	Pa×s	1093.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116345972&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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