

Diphenacyl isophthalate

Inchi:	InChI=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/molxK	1093.86	Joback Method
cpg	920.13	J/molxK	1136.84	Joback Method
cpg	925.77	J/molxK	1179.82	Joback Method
cpg	930.04	J/molxK	1222.80	Joback Method
cpg	933.01	J/molxK	1265.78	Joback Method
cpg	934.77	J/molxK	1308.77	Joback Method
cpg	935.41	J/molxK	1351.75	Joback Method
dvisc	0.0002189	Paxs	696.20	Joback Method
dvisc	0.0001354	Paxs	762.48	Joback Method

dvisc	0.0000904	Paxs	828.75	Joback Method
dvisc	0.0000641	Paxs	895.03	Joback Method
dvisc	0.0000477	Paxs	961.31	Joback Method
dvisc	0.0000368	Paxs	1027.58	Joback Method
dvisc	0.0000293	Paxs	1093.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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