

Isophthalic acid, 2,5-dimethylphenyl ethyl ester

Inchi:	InChI=1S/C18H18O4/c1-4-21-17(19)14-6-5-7-15(11-14)18(20)22-16-10-12(2)8-9-13(16)3
InchiKey:	WSQSJFBCVLXBIA-UHFFFAOYSA-N
Formula:	C18H18O4
SMILES:	CCOC(=O)c1cccc(C(=O)Oc2cc(C)ccc2C)c1
Mol. weight [g/mol]:	298.33

Physical Properties

Property code	Value	Unit	Source
gf	-171.23	kJ/mol	Joback Method
hf	-465.80	kJ/mol	Joback Method
hfus	34.86	kJ/mol	Joback Method
hvap	80.51	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	3.699		Crippen Method
mcvol	231.840	ml/mol	McGowan Method
pc	1998.33	kPa	Joback Method
rinsol	2430.00		NIST Webbook
tb	832.12	K	Joback Method
tc	1062.20	K	Joback Method
tf	527.34	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.72	J/molxK	832.12	Joback Method
cpg	679.47	J/molxK	870.47	Joback Method
cpg	691.98	J/molxK	908.81	Joback Method
cpg	703.26	J/molxK	947.16	Joback Method
cpg	713.33	J/molxK	985.51	Joback Method
cpg	722.22	J/molxK	1023.86	Joback Method
cpg	729.93	J/molxK	1062.20	Joback Method
dvisc	0.0004755	Paxs	527.34	Joback Method
dvisc	0.0003055	Paxs	578.14	Joback Method

dvisc	0.0002108	Paxs	628.93	Joback Method
dvisc	0.0001538	Paxs	679.73	Joback Method
dvisc	0.0001172	Paxs	730.53	Joback Method
dvisc	0.0000925	Paxs	781.32	Joback Method
dvisc	0.0000752	Paxs	832.12	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=U344539&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
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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