

Isophthalic acid, dineopentyl ester

Inchi:	InChI=1S/C18H26O4/c1-17(2,3)11-21-15(19)13-8-7-9-14(10-13)16(20)22-12-18(4,5)6/h7
InchiKey:	WYEHFCKMWFUROQ-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CC(C)(C)COC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-258.70	kJ/mol	Joback Method
hf	-696.89	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.092		Crippen Method
mvol	255.600	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2096.00		NIST Webbook
rinpol	2096.00		NIST Webbook
tb	789.02	K	Joback Method
tc	1003.92	K	Joback Method
tf	480.72	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.44	J/molxK	789.02	Joback Method
cpg	834.56	J/molxK	968.11	Joback Method
cpg	822.66	J/molxK	932.29	Joback Method
cpg	809.75	J/molxK	896.47	Joback Method
cpg	795.79	J/molxK	860.65	Joback Method
cpg	780.71	J/molxK	824.84	Joback Method
cpg	845.53	J/molxK	1003.92	Joback Method
dvisc	0.0000468	Paxs	789.02	Joback Method

dvisc	0.0000621	Paxs	737.64	Joback Method
dvisc	0.0000860	Paxs	686.25	Joback Method
dvisc	0.0001256	Paxs	634.87	Joback Method
dvisc	0.0001959	Paxs	583.49	Joback Method
dvisc	0.0003329	Paxs	532.10	Joback Method
dvisc	0.0006338	Paxs	480.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343875&Units=SI
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

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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