

Isophthalic acid, 2-methylphenyl nonyl ester

Inchi:	InChI=1S/C24H30O4/c1-3-4-5-6-7-8-11-17-27-23(25)20-14-12-15-21(18-20)24(26)28-22
InchiKey:	YBEDUQRVBJAEOF-UHFFFAOYSA-N
Formula:	C24H30O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)Oc2ccccc2C)c1
Mol. weight [g/mol]:	382.49

Physical Properties

Property code	Value	Unit	Source
gf	-111.08	kJ/mol	Joback Method
hf	-578.17	kJ/mol	Joback Method
hfus	50.79	kJ/mol	Joback Method
hvap	93.21	kJ/mol	Joback Method
log10ws	-7.63		Crippen Method
logp	6.122		Crippen Method
mvol	316.380	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	3062.00		NIST Webbook
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tb	964.42	K	Joback Method
tc	1187.99	K	Joback Method
tf	582.44	K	Joback Method
vc	1.212	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.71	J/molxK	964.42	Joback Method
cpg	1073.72	J/molxK	1150.73	Joback Method
cpg	1064.74	J/molxK	1113.47	Joback Method
cpg	1054.50	J/molxK	1076.21	Joback Method
cpg	1042.95	J/molxK	1038.94	Joback Method
cpg	1030.03	J/molxK	1001.68	Joback Method
cpg	1081.47	J/molxK	1187.99	Joback Method
dvisc	0.0000325	Paxs	964.42	Joback Method

dvisc	0.0000413	Paxs	900.76	Joback Method
dvisc	0.0000545	Paxs	837.09	Joback Method
dvisc	0.0000752	Paxs	773.43	Joback Method
dvisc	0.0001098	Paxs	709.77	Joback Method
dvisc	0.0001730	Paxs	646.10	Joback Method
dvisc	0.0003008	Paxs	582.44	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=U344352&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_cvol:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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