

Isophthalic acid, neopentyl nonyl ester

Inchi:	InChI=1S/C22H34O4/c1-5-6-7-8-9-10-11-15-25-20(23)18-13-12-14-19(16-18)21(24)26-1
InchiKey:	GCSLDJWHOZJSFT-UHFFFAOYSA-N
Formula:	C22H34O4
SMILES:	CCCCCCCCCOC(=O)c1cccc(C(=O)OCC(C)(C)C)c1
Mol. weight [g/mol]:	362.50

Physical Properties

Property code	Value	Unit	Source
gf	-227.86	kJ/mol	Joback Method
hf	-770.70	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	5.797		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2623.00		NIST Webbook
tb	883.77	K	Joback Method
tc	1090.17	K	Joback Method
tf	523.38	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.84	J/molxK	883.77	Joback Method
cpg	1069.39	J/molxK	1055.77	Joback Method
cpg	1057.31	J/molxK	1021.37	Joback Method
cpg	1044.16	J/molxK	986.97	Joback Method
cpg	1029.90	J/molxK	952.57	Joback Method
cpg	1014.47	J/molxK	918.17	Joback Method
cpg	1080.45	J/molxK	1090.17	Joback Method
dvisc	0.0000322	Paxs	883.77	Joback Method
dvisc	0.0000424	Paxs	823.70	Joback Method

dvisc	0.0000583	Paxs	763.64	Joback Method
dvisc	0.0000847	Paxs	703.57	Joback Method
dvisc	0.0001320	Paxs	643.51	Joback Method
dvisc	0.0002253	Paxs	583.44	Joback Method
dvisc	0.0004346	Paxs	523.38	Joback Method

Sources

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=U343867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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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