

Isophthalic acid, cis-hex-3-enyl nonyl ester

Inchi:	InChI=1S/C23H34O4/c1-3-5-7-9-10-11-13-18-27-23(25)21-16-14-15-20(19-21)22(24)26-
InchiKey:	UOINNQINQRTPH-VURMDHGXSA-N
Formula:	C23H34O4
SMILES:	CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCC)c1
Mol. weight [g/mol]:	374.51

Physical Properties

Property code	Value	Unit	Source
gf	-142.06	kJ/mol	Joback Method
hf	-665.37	kJ/mol	Joback Method
hfus	54.75	kJ/mol	Joback Method
hvap	88.00	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	6.107		Crippen Method
mcvol	321.750	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	2748.00		NIST Webbook
tb	914.04	K	Joback Method
tc	1122.42	K	Joback Method
tf	527.15	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.46	J/molxK	914.04	Joback Method
cpg	1046.83	J/molxK	948.77	Joback Method
cpg	1062.01	J/molxK	983.50	Joback Method
cpg	1076.03	J/molxK	1018.23	Joback Method
cpg	1088.95	J/molxK	1052.96	Joback Method
cpg	1100.82	J/molxK	1087.69	Joback Method
cpg	1111.67	J/molxK	1122.42	Joback Method
dvisc	0.0003985	Paxs	527.15	Joback Method
dvisc	0.0002069	Paxs	591.63	Joback Method

dvisc	0.0001222	Paxs	656.11	Joback Method
dvisc	0.0000793	Paxs	720.59	Joback Method
dvisc	0.0000552	Paxs	785.08	Joback Method
dvisc	0.0000406	Paxs	849.56	Joback Method
dvisc	0.0000312	Paxs	914.04	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=U356703&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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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