

Terephthalic acid, 3-hexyl isoheptyl ester

Inchi:	InChI=1S/C20H30O4/c1-5-8-18(6-2)24-20(22)17-12-10-16(11-13-17)19(21)23-14-7-9-15
InchiKey:	KRFYQTJUVXBRRN-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CCCC(CC)OC(=O)c1ccc(C(=O)OCCCC(C)C)cc1
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-252.42	kJ/mol	Joback Method
hf	-731.23	kJ/mol	Joback Method
hfus	39.74	kJ/mol	Joback Method
hvap	80.59	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.015		Crippen Method
mvol	283.780	ml/mol	McGowan Method
pc	1357.63	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	840.36	K	Joback Method
tc	1043.99	K	Joback Method
tf	468.42	K	Joback Method
vc	1.083	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.75	J/molxK	840.36	Joback Method
cpg	895.15	J/molxK	874.30	Joback Method
cpg	910.36	J/molxK	908.24	Joback Method
cpg	924.40	J/molxK	942.18	Joback Method
cpg	937.29	J/molxK	976.12	Joback Method
cpg	949.07	J/molxK	1010.06	Joback Method
cpg	959.75	J/molxK	1043.99	Joback Method
dvisc	0.0007750	Paxs	468.42	Joback Method

dvisc	0.0003677	Paxs	530.41	Joback Method
dvisc	0.0002040	Paxs	592.40	Joback Method
dvisc	0.0001265	Paxs	654.39	Joback Method
dvisc	0.0000852	Paxs	716.38	Joback Method
dvisc	0.0000611	Paxs	778.37	Joback Method
dvisc	0.0000460	Paxs	840.36	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=U356228&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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