

Terephthalic acid, hexyl 2-phenoxyethyl ester

Inchi:	InChI=1S/C22H26O5/c1-2-3-4-8-15-26-21(23)18-11-13-19(14-12-18)22(24)27-17-16-25-
InchiKey:	FFIFSYUMKUTQDM-UHFFFAOYSA-N
Formula:	C22H26O5
SMILES:	CCCCCOC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1
Mol. weight [g/mol]:	370.44

Physical Properties

Property code	Value	Unit	Source
gf	-223.29	kJ/mol	Joback Method
hf	-657.64	kJ/mol	Joback Method
hfus	47.19	kJ/mol	Joback Method
hvap	90.50	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	4.659		Crippen Method
mvol	294.070	ml/mol	McGowan Method
pc	1470.23	kPa	Joback Method
rinpol	3054.00		NIST Webbook
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tb	936.10	K	Joback Method
tc	1158.31	K	Joback Method
tf	569.61	K	Joback Method
vc	1.117	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.35	J/molxK	936.10	Joback Method
cpg	938.87	J/molxK	973.14	Joback Method
cpg	950.95	J/molxK	1010.17	Joback Method
cpg	961.63	J/molxK	1047.21	Joback Method
cpg	970.94	J/molxK	1084.24	Joback Method
cpg	978.89	J/molxK	1121.28	Joback Method
cpg	985.53	J/molxK	1158.31	Joback Method
dvisc	0.0002967	Paxs	569.61	Joback Method

dvisc	0.0001706	Paxs	630.69	Joback Method
dvisc	0.0001081	Paxs	691.77	Joback Method
dvisc	0.0000738	Paxs	752.86	Joback Method
dvisc	0.0000533	Paxs	813.94	Joback Method
dvisc	0.0000403	Paxs	875.02	Joback Method
dvisc	0.0000316	Paxs	936.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416045&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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