

Terephthalic acid, 2-phenoxyethyl propyl ester

Inchi:	InChI=1S/C19H20O5/c1-2-12-23-18(20)15-8-10-16(11-9-15)19(21)24-14-13-22-17-6-4-3
InchiKey:	MXSLLNMGOXPAKV-UHFFFAOYSA-N
Formula:	C19H20O5
SMILES:	CCCOC(=O)c1ccc(C(=O)OCCOc2ccccc2)cc1
Mol. weight [g/mol]:	328.36

Physical Properties

Property code	Value	Unit	Source
gf	-248.55	kJ/mol	Joback Method
hf	-595.72	kJ/mol	Joback Method
hfus	39.42	kJ/mol	Joback Method
hvap	83.82	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.489		Crippen Method
mcvol	251.800	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinsol	2675.00		NIST Webbook
tb	867.46	K	Joback Method
tc	1091.97	K	Joback Method
tf	535.80	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	751.41	J/molxK	867.46	Joback Method
cpg	764.83	J/molxK	904.88	Joback Method
cpg	776.93	J/molxK	942.30	Joback Method
cpg	787.70	J/molxK	979.72	Joback Method
cpg	797.19	J/molxK	1017.14	Joback Method
cpg	805.39	J/molxK	1054.56	Joback Method
cpg	812.34	J/molxK	1091.97	Joback Method
dvisc	0.0004045	Paxs	535.80	Joback Method
dvisc	0.0002407	Paxs	591.08	Joback Method

dvisc	0.0001566	Paxs	646.35	Joback Method
dvisc	0.0001090	Paxs	701.63	Joback Method
dvisc	0.0000799	Paxs	756.91	Joback Method
dvisc	0.0000612	Paxs	812.18	Joback Method
dvisc	0.0000485	Paxs	867.46	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=U416041&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
mccvol:	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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