

Phthalic acid, isobutyl 2-phenoxyethyl ester

Inchi: InChI=1S/C20H22O5/c1-15(2)14-25-20(22)18-11-7-6-10-17(18)19(21)24-13-12-23-16-8-
InchiKey: ZQEPAAJFYDBHML-UHFFFAOYSA-N
Formula: C20H22O5
SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCCOc1ccccc1
Mol. weight [g/mol]: 342.39

Physical Properties

Property code	Value	Unit	Source
gf	-242.57	kJ/mol	Joback Method
hf	-621.64	kJ/mol	Joback Method
hfus	38.49	kJ/mol	Joback Method
hvap	85.66	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.735		Crippen Method
mcvol	265.890	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook
tb	889.90	K	Joback Method
tc	1115.53	K	Joback Method
tf	532.07	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	809.26	J/molxK	889.90	Joback Method
cpg	822.86	J/molxK	927.51	Joback Method
cpg	835.06	J/molxK	965.11	Joback Method
cpg	845.87	J/molxK	1002.72	Joback Method
cpg	855.32	J/molxK	1040.32	Joback Method
cpg	863.42	J/molxK	1077.93	Joback Method
cpg	870.21	J/molxK	1115.53	Joback Method
dvisc	0.0004028	Paxs	532.07	Joback Method

dvisc	0.0002237	Paxs	591.71	Joback Method
dvisc	0.0001383	Paxs	651.35	Joback Method
dvisc	0.0000927	Paxs	710.99	Joback Method
dvisc	0.0000661	Paxs	770.62	Joback Method
dvisc	0.0000495	Paxs	830.26	Joback Method
dvisc	0.0000385	Paxs	889.90	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=U382479&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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