

Phthalic acid, hexyl 2-methylbenzyl ester

Inchi:	InChI=1S/C22H26O4/c1-3-4-5-10-15-25-21(23)19-13-8-9-14-20(19)22(24)26-16-18-12-7
InchiKey:	AQURXDGIDLTBQQ-UHFFFAOYSA-N
Formula:	C22H26O4
SMILES:	CCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C
Mol. weight [g/mol]:	354.44

Physical Properties

Property code	Value	Unit	Source
gf	-127.92	kJ/mol	Joback Method
hf	-536.89	kJ/mol	Joback Method
hfus	45.61	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.089		Crippen Method
mvol	288.200	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook
tb	918.66	K	Joback Method
tc	1141.14	K	Joback Method
tf	559.90	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.78	J/molxK	918.66	Joback Method
cpg	911.00	J/molxK	955.74	Joback Method
cpg	923.89	J/molxK	992.82	Joback Method
cpg	935.48	J/molxK	1029.90	Joback Method
cpg	945.81	J/molxK	1066.98	Joback Method
cpg	954.92	J/molxK	1104.06	Joback Method
cpg	962.84	J/molxK	1141.14	Joback Method
dvisc	0.0003717	Paxs	559.90	Joback Method

dvisc	0.0002185	Paxs	619.69	Joback Method
dvisc	0.0001410	Paxs	679.49	Joback Method
dvisc	0.0000977	Paxs	739.28	Joback Method
dvisc	0.0000715	Paxs	799.07	Joback Method
dvisc	0.0000547	Paxs	858.87	Joback Method
dvisc	0.0000433	Paxs	918.66	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=U382852&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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