Dineopentyl phthalate

Other names:	1,2-Benzenedicarboxylic acid, dineopentyl ester
	Dineopentyl-1,2-benzenedicarboxylate
Inchi:	InChI=1S/C18H26O4/c1-17(2,3)11-21-15(19)13-9-7-8-10-14(13)16(20)22-12-18(4,5)6/h7
InchiKey:	GAHSOBODSWGWHR-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CC(C)(C)COC(=O)c1ccccc1C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	306.40
CAS:	2553-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-258.70	kJ/mol	Joback Method
hf	-696.89	kJ/mol	Joback Method
hfus	26.77	kJ/mol	Joback Method
hvap	74.32	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.092		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	1938.00		NIST Webbook
tb	789.02	K	Joback Method
tc	1003.92	K	Joback Method
tf	480.72	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.44	J/mol×K	789.02	Joback Method
cpg	834.56	J/mol×K	968.11	Joback Method
cpg	822.66	J/mol×K	932.29	Joback Method
cpg	809.75	J/mol×K	896.47	Joback Method
cpg	795.79	J/mol×K	860.65	Joback Method
cpg	780.71	J/mol×K	824.84	Joback Method

cpg	845.53	J/mol×K	1003.92	Joback Method
dvisc	0.0000468	Pa×s	789.02	Joback Method
dvisc	0.0000621	Pa×s	737.64	Joback Method
dvisc	0.0000860	Pa×s	686.25	Joback Method
dvisc	0.0001256	Pa×s	634.87	Joback Method
dvisc	0.0001959	Pa×s	583.49	Joback Method
dvisc	0.0003329	Pa×s	532.10	Joback Method
dvisc	0.0006338	Pa×s	480.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C2553244&Units=SI

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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