

1,3-Benzenedicarboxylic acid, dipentyl ester

Inchi:	InChI=1S/C18H26O4/c1-3-5-7-12-21-17(19)15-10-9-11-16(14-15)18(20)22-13-8-6-4-2/h
InchiKey:	KHVWJDHKBKQEWMR-UHFFFAOYSA-N
Formula:	C18H26O4
SMILES:	CCCCOC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]:	306.40

Physical Properties

Property code	Value	Unit	Source
gf	-264.38	kJ/mol	Joback Method
hf	-679.39	kJ/mol	Joback Method
hfus	41.60	kJ/mol	Joback Method
hvap	76.91	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.381		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1552.45	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
rinpol	2219.00		NIST Webbook
tb	795.48	K	Joback Method
tc	995.15	K	Joback Method
tf	475.88	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.25	J/molxK	795.48	Joback Method
cpg	776.92	J/molxK	828.76	Joback Method
cpg	791.55	J/molxK	862.04	Joback Method
cpg	805.16	J/molxK	895.32	Joback Method
cpg	817.75	J/molxK	928.59	Joback Method
cpg	829.35	J/molxK	961.87	Joback Method

cpg	839.97	J/mol×K	995.15	Joback Method
dvisc	0.0007181	Paxs	475.88	Joback Method
dvisc	0.0004036	Paxs	529.15	Joback Method
dvisc	0.0002520	Paxs	582.41	Joback Method
dvisc	0.0001703	Paxs	635.68	Joback Method
dvisc	0.0001223	Paxs	688.95	Joback Method
dvisc	0.0000921	Paxs	742.21	Joback Method
dvisc	0.0000720	Paxs	795.48	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=R15123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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