Dibutyl isophthalate

Other names: 1,3-Benzenedicarboxylic acid, dibutyl ester
Isophthalic acid, dibutyl ester
Inchi: InChI=1S/C16H22O4/c1-3-5-10-19-15(17)13-8-7-9-14(12-13)16(18)20-11-6-4-2/h7-9,12H
InchiKey: GOPWOUQJIMLDDM-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCCOC(=O)c1cccc(C(=O)OCCCC)c1
Mol. weight [g/mol]: 278.34
CAS: 3126-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-281.22	kJ/mol	Joback Method
hf	-638.11	kJ/mol	Joback Method
hfus	36.42	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.600		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	1996.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	749.72	K	Joback Method
tc	951.49	K	Joback Method
tf	453.34	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/mol×K	749.72	Joback Method
cpg	663.58	J/mol×K	783.35	Joback Method
cpg	677.73	J/mol×K	816.98	Joback Method
cpg	690.92	J/mol×K	850.61	Joback Method
cpg	703.17	J/mol×K	884.24	Joback Method
cpg	714.48	J/mol×K	917.86	Joback Method
cpg	724.87	J/mol×K	951.49	Joback Method
dvisc	0.0008522	Pa×s	453.34	Joback Method
dvisc	0.0004919	Pa×s	502.74	Joback Method
dvisc	0.0003132	Pa×s	552.13	Joback Method
dvisc	0.0002148	Pa×s	601.53	Joback Method
dvisc	0.0001560	Pa×s	650.93	Joback Method
dvisc	0.0001185	Pa×s	700.32	Joback Method
dvisc	0.0000934	Pa×s	749.72	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=C3126907&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