

Phthalic acid, butyl 3-iodobenzyl ester

Inchi:	InChI=1S/C19H19IO4/c1-2-3-11-23-18(21)16-9-4-5-10-17(16)19(22)24-13-14-7-6-8-15(2
InchiKey:	XYBMUFRHCBHSGY-UHFFFAOYSA-N
Formula:	C19H19IO4
SMILES:	CCCCOC(=O)c1ccccc1C(=O)OCc1cccc(I)c1
Mol. weight [g/mol]:	438.26

Physical Properties

Property code	Value	Unit	Source
gf	-95.06	kJ/mol	Joback Method
hf	-398.10	kJ/mol	Joback Method
hfus	42.25	kJ/mol	Joback Method
hvap	91.45	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.605		Crippen Method
mcvol	271.750	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2805.00		NIST Webbook
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tb	943.16	K	Joback Method
tc	1189.04	K	Joback Method
tf	584.15	K	Joback Method
vc	1.020	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.00	J/molxK	943.16	Joback Method
cpg	810.34	J/molxK	1148.06	Joback Method
cpg	803.62	J/molxK	1107.08	Joback Method
cpg	795.78	J/molxK	1066.10	Joback Method
cpg	786.76	J/molxK	1025.12	Joback Method
cpg	776.52	J/molxK	984.14	Joback Method
cpg	815.99	J/molxK	1189.04	Joback Method
dvisc	0.0000476	Paxs	943.16	Joback Method

dvisc	0.0000597	Paxs	883.33	Joback Method
dvisc	0.0000774	Paxs	823.49	Joback Method
dvisc	0.0001046	Paxs	763.65	Joback Method
dvisc	0.0001486	Paxs	703.82	Joback Method
dvisc	0.0002254	Paxs	643.99	Joback Method
dvisc	0.0003723	Paxs	584.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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