

Phthalic acid, 8-bromooctyl pentyl ester

Inchi:	InChI=1S/C21H31BrO4/c1-2-3-11-16-25-20(23)18-13-8-9-14-19(18)21(24)26-17-12-7-5-
InchiKey:	MRXMUEKELMWPJB-UHFFFAOYSA-N
Formula:	C21H31BrO4
SMILES:	CCCCCOC(=O)c1cccc1C(=O)OCCCCCCCCBr
Mol. weight [g/mol]:	427.37

Physical Properties

Property code	Value	Unit	Source
gf	-224.80	kJ/mol	Joback Method
hf	-714.98	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.926		Crippen Method
mvol	315.370	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	3269.00		NIST Webbook
rinpol	3269.00		NIST Webbook
tb	930.28	K	Joback Method
tc	1143.52	K	Joback Method
tf	569.49	K	Joback Method
vc	1.214	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.64	J/molxK	930.28	Joback Method
cpg	992.30	J/molxK	965.82	Joback Method
cpg	1005.78	J/molxK	1001.36	Joback Method
cpg	1018.09	J/molxK	1036.90	Joback Method
cpg	1029.29	J/molxK	1072.44	Joback Method
cpg	1039.42	J/molxK	1107.98	Joback Method
cpg	1048.51	J/molxK	1143.52	Joback Method
dvisc	0.0003471	Paxs	569.49	Joback Method

dvisc	0.0001999	Paxs	629.62	Joback Method
dvisc	0.0001267	Paxs	689.75	Joback Method
dvisc	0.0000864	Paxs	749.88	Joback Method
dvisc	0.0000624	Paxs	810.02	Joback Method
dvisc	0.0000471	Paxs	870.15	Joback Method
dvisc	0.0000369	Paxs	930.28	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=U382555&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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