

Phthalic acid, 7-bromoheptyl pentyl ester

Inchi:	InChI=1S/C20H29BrO4/c1-2-3-10-15-24-19(22)17-12-7-8-13-18(17)20(23)25-16-11-6-4-5
InchiKey:	MOEASUZEFMZIGG-UHFFFAOYSA-N
Formula:	C20H29BrO4
SMILES:	CCCCCOC(=O)c1cccc1C(=O)OCCCCCBr
Mol. weight [g/mol]:	413.35

Physical Properties

Property code	Value	Unit	Source
gf	-233.22	kJ/mol	Joback Method
hf	-694.34	kJ/mol	Joback Method
hfus	52.07	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.536		Crippen Method
mvol	301.280	ml/mol	McGowan Method
pc	1412.25	kPa	Joback Method
rinpol	2965.00		NIST Webbook
rinpol	2965.00		NIST Webbook
tb	907.40	K	Joback Method
tc	1118.87	K	Joback Method
tf	558.22	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.16	J/molxK	907.40	Joback Method
cpg	979.30	J/molxK	1083.62	Joback Method
cpg	969.22	J/molxK	1048.38	Joback Method
cpg	958.11	J/molxK	1013.13	Joback Method
cpg	945.91	J/molxK	977.89	Joback Method
cpg	932.61	J/molxK	942.64	Joback Method
cpg	988.36	J/molxK	1118.87	Joback Method
dvisc	0.0000429	Paxs	907.40	Joback Method

dvisc	0.0000546	Paxs	849.20	Joback Method
dvisc	0.0000721	Paxs	791.01	Joback Method
dvisc	0.0000994	Paxs	732.81	Joback Method
dvisc	0.0001448	Paxs	674.61	Joback Method
dvisc	0.0002264	Paxs	616.42	Joback Method
dvisc	0.0003888	Paxs	558.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415519&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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