

Terephthalic acid, 2-bromobenzyl hexyl ester

Inchi:	InChI=1S/C21H23BrO4/c1-2-3-4-7-14-25-20(23)16-10-12-17(13-11-16)21(24)26-15-18-8
InchiKey:	XEWIYTKZJXVEAE-UHFFFAOYSA-N
Formula:	C21H23BrO4
SMILES:	CCCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2Br)cc1
Mol. weight [g/mol]:	419.31

Physical Properties

Property code	Value	Unit	Source
gf	-122.02	kJ/mol	Joback Method
hf	-489.92	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	92.96	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.543		Crippen Method
mcvol	291.610	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	3158.00		NIST Webbook
rinpol	3158.00		NIST Webbook
tb	961.94	K	Joback Method
tc	1195.16	K	Joback Method
tf	608.43	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.72	J/molxK	961.94	Joback Method
cpg	883.96	J/molxK	1000.81	Joback Method
cpg	894.93	J/molxK	1039.68	Joback Method
cpg	904.68	J/molxK	1078.55	Joback Method
cpg	913.26	J/molxK	1117.42	Joback Method
cpg	920.74	J/molxK	1156.29	Joback Method
cpg	927.15	J/molxK	1195.16	Joback Method
dvisc	0.0002818	Paxs	608.43	Joback Method

dvisc	0.0001753	Paxs	667.35	Joback Method
dvisc	0.0001177	Paxs	726.27	Joback Method
dvisc	0.0000839	Paxs	785.18	Joback Method
dvisc	0.0000628	Paxs	844.10	Joback Method
dvisc	0.0000487	Paxs	903.02	Joback Method
dvisc	0.0000390	Paxs	961.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416082&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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