

Terephthalic acid, 2-bromobenzyl octyl ester

Inchi: InChI=1S/C23H27BrO4/c1-2-3-4-5-6-9-16-27-22(25)18-12-14-19(15-13-18)23(26)28-17-2
InchiKey: MOPJWL0DXSGVCF-UHFFFAOYSA-N
Formula: C23H27BrO4
SMILES: CCCCCCOC(=O)c1ccc(C(=O)OCc2ccccc2Br)cc1
Mol. weight [g/mol]: 447.36

Physical Properties

Property code	Value	Unit	Source
gf	-105.18	kJ/mol	Joback Method
hf	-531.20	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	97.42	kJ/mol	Joback Method
log10ws	-8.16		Crippen Method
logp	6.323		Crippen Method
mcvol	319.790	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2856.00		NIST Webbook
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tb	1007.70	K	Joback Method
tc	1241.48	K	Joback Method
tf	630.97	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.51	J/molxK	1007.70	Joback Method
cpg	1038.96	J/molxK	1202.51	Joback Method
cpg	1031.46	J/molxK	1163.55	Joback Method
cpg	1022.83	J/molxK	1124.59	Joback Method
cpg	1013.00	J/molxK	1085.63	Joback Method
cpg	1001.91	J/molxK	1046.66	Joback Method
cpg	1045.39	J/molxK	1241.48	Joback Method
dvisc	0.0000289	Paxs	1007.70	Joback Method

dvisc	0.0000363	Paxs	944.91	Joback Method
dvisc	0.0000471	Paxs	882.12	Joback Method
dvisc	0.0000636	Paxs	819.34	Joback Method
dvisc	0.0000903	Paxs	756.55	Joback Method
dvisc	0.0001367	Paxs	693.76	Joback Method
dvisc	0.0002246	Paxs	630.97	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=U416084&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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