

Terephthalic acid, 3-bromobenzyl heptyl ester

Inchi:	InChI=1S/C22H25BrO4/c1-2-3-4-5-6-14-26-21(24)18-10-12-19(13-11-18)22(25)27-16-17
InchiKey:	QDLWXRPCXLKUEG-UHFFFAOYSA-N
Formula:	C22H25BrO4
SMILES:	CCCCCCCOC(=O)c1ccc(C(=O)OCc2cccc(Br)c2)cc1
Mol. weight [g/mol]:	433.34

Physical Properties

Property code	Value	Unit	Source
gf	-113.60	kJ/mol	Joback Method
hf	-510.56	kJ/mol	Joback Method
hfus	50.90	kJ/mol	Joback Method
hvap	95.19	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	5.933		Crippen Method
mcvol	305.700	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	3517.00		NIST Webbook
rinpol	3517.00		NIST Webbook
tb	984.82	K	Joback Method
tc	1217.88	K	Joback Method
tf	619.70	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.34	J/molxK	984.82	Joback Method
cpg	942.66	J/molxK	1023.66	Joback Method
cpg	953.69	J/molxK	1062.51	Joback Method
cpg	963.48	J/molxK	1101.35	Joback Method
cpg	972.10	J/molxK	1140.19	Joback Method
cpg	979.60	J/molxK	1179.04	Joback Method
cpg	986.02	J/molxK	1217.88	Joback Method
dvisc	0.0002520	Paxs	619.70	Joback Method

dvisc	0.0001550	Paxs	680.55	Joback Method
dvisc	0.0001033	Paxs	741.41	Joback Method
dvisc	0.0000732	Paxs	802.26	Joback Method
dvisc	0.0000544	Paxs	863.11	Joback Method
dvisc	0.0000421	Paxs	923.97	Joback Method
dvisc	0.0000336	Paxs	984.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383025&Units=SI

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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