

Terephthalic acid, 3-bromobenzyl ethyl ester

Inchi: InChI=1S/C17H15BrO4/c1-2-21-16(19)13-6-8-14(9-7-13)17(20)22-11-12-4-3-5-15(18)10
InchiKey: USBKEGGACWAKMK-UHFFFAOYSA-N
Formula: C17H15BrO4
SMILES: CCOC(=O)c1ccc(C(=O)OCc2cccc(Br)c2)cc1
Mol. weight [g/mol]: 363.20

Physical Properties

Property code	Value	Unit	Source
gf	-155.70	kJ/mol	Joback Method
hf	-407.36	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	84.06	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	3.983		Crippen Method
mcvol	235.250	ml/mol	McGowan Method
pc	2363.37	kPa	Joback Method
rinpol	3003.00		NIST Webbook
rinpol	3003.00		NIST Webbook
tb	870.42	K	Joback Method
tc	1112.19	K	Joback Method
tf	563.35	K	Joback Method
vc	0.881	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.96	J/molxK	870.42	Joback Method
cpg	655.66	J/molxK	910.71	Joback Method
cpg	666.16	J/molxK	951.01	Joback Method
cpg	675.49	J/molxK	991.30	Joback Method
cpg	683.69	J/molxK	1031.60	Joback Method
cpg	690.80	J/molxK	1071.89	Joback Method
cpg	696.86	J/molxK	1112.19	Joback Method
dvisc	0.0004265	Paxs	563.35	Joback Method

dvisc	0.0002779	Paxs	614.53	Joback Method
dvisc	0.0001934	Paxs	665.71	Joback Method
dvisc	0.0001418	Paxs	716.88	Joback Method
dvisc	0.0001083	Paxs	768.06	Joback Method
dvisc	0.0000856	Paxs	819.24	Joback Method
dvisc	0.0000695	Paxs	870.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383019&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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