Terephthalic acid, 3-bromobenzyl propyl ester

Inchi: InChI=1S/C18H17BrO4/c1-2-10-22-17(20)14-6-8-15(9-7-14)18(21)23-12-13-4-3-5-16(19)
InchiKey: GNFJGFAWBOTCKT-UHFFFAOYSA-N
Formula: C18H17BrO4
SMILES: CCCOC(=O)c1ccc(C(=O)OCc2cccc(Br)c2)cc1
Mol. weight [g/mol]: 377.23

Physical Properties

Property code	Value	Unit	Source
gf	-147.28	kJ/mol	Joback Method
hf	-428.00	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.373		Crippen Method
mcvol	249.340	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	3107.00		NIST Webbook
rinpol	3107.00		NIST Webbook
tb	893.30	K	Joback Method
tc	1131.83	K	Joback Method
tf	574.62	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.78	J/mol×K	893.30	Joback Method
cpg	711.67	J/mol×K	933.06	Joback Method
cpg	722.33	J/mol×K	972.81	Joback Method
cpg	731.82	J/mol×K	1012.57	Joback Method
cpg	740.17	J/mol×K	1052.32	Joback Method
cpg	747.42	J/mol×K	1092.08	Joback Method
cpg	753.62	J/mol×K	1131.83	Joback Method
dvisc	0.0003867	Pa×s	574.62	Joback Method

dvisc	0.0002489	Pa×s	627.73	Joback Method
dvisc	0.0001716	Pa×s	680.85	Joback Method
dvisc	0.0001249	Pa×s	733.96	Joback Method
dvisc	0.0000949	Pa×s	787.07	Joback Method
dvisc	0.0000746	Pa×s	840.19	Joback Method
dvisc	0.0000604	Pa×s	893.30	Joback Method

Sources

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=U383020&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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