Glutaric acid, 4-bromophenyl heptyl ester

Inchi: InChI=1S/C18H25BrO4/c1-2-3-4-5-6-14-22-17(20)8-7-9-18(21)23-16-12-10-15(19)11-13-
InchiKey: JKQJFSYAMHUMOS-UHFFFAOYSA-N
Formula: C18H25BrO4
SMILES: CCCCCCCOC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 385.29

Physical Properties

Property code	Value	Unit	Source
gf	-250.06	kJ/mol	Joback Method
hf	-653.06	kJ/mol	Joback Method
hfus	46.89	kJ/mol	Joback Method
hvap	83.35	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.038		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1640.43	kPa	Joback Method
rinpol	2638.00		NIST Webbook
rinpol	2638.00		NIST Webbook
tb	861.64	K	Joback Method
tc	1071.94	K	Joback Method
tf	535.68	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	801.28	J/mol×K	861.64	Joback Method
cpg	860.97	J/mol×K	1036.89	Joback Method
cpg	851.06	J/mol×K	1001.84	Joback Method
cpg	840.16	J/mol×K	966.79	Joback Method
cpg	828.25	J/mol×K	931.74	Joback Method
cpg	815.30	J/mol×K	896.69	Joback Method
cpg	869.92	J/mol×K	1071.94	Joback Method
dvisc	0.0000577	Pa×s	861.64	Joback Method

dvisc	0.0000730	Pa×s	807.31	Joback Method
dvisc	0.0000955	Pa×s	752.99	Joback Method
dvisc	0.0001303	Pa×s	698.66	Joback Method
dvisc	0.0001874	Pa×s	644.33	Joback Method
dvisc	0.0002881	Pa×s	590.01	Joback Method
dvisc	0.0004832	Pa×s	535.68	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=U358726&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