Glutaric acid, 4-bromophenyl tetradecyl ester

Inchi: InChI=1S/C25H39BrO4/c1-2-3-4-5-6-7-8-9-10-11-12-13-21-29-24(27)15-14-16-25(28)30-
InchiKey: ALERBYXXZFUSJD-UHFFFAOYSA-N
Formula: C25H39BrO4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 483.48

Physical Properties

Property code	Value	Unit	Source
gf	-191.12	kJ/mol	Joback Method
hf	-797.54	kJ/mol	Joback Method
hfus	65.02	kJ/mol	Joback Method
hvap	98.93	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.769		Crippen Method
mcvol	371.730	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	3397.00		NIST Webbook
rinpol	3397.00		NIST Webbook
tb	1021.80	K	Joback Method
tc	1251.48	K	Joback Method
tf	614.57	K	Joback Method
vc	1.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.24	J/mol×K	1021.80	Joback Method
cpg	1236.89	J/mol×K	1060.08	Joback Method
cpg	1251.09	J/mol×K	1098.36	Joback Method
cpg	1263.89	J/mol×K	1136.64	Joback Method
cpg	1275.36	J/mol×K	1174.92	Joback Method
cpg	1285.57	J/mol×K	1213.20	Joback Method
cpg	1294.58	J/mol×K	1251.48	Joback Method
dvisc	0.0002140	Pa×s	614.57	Joback Method

dvisc	0.0001182	Pa×s	682.44	Joback Method
dvisc	0.0000727	Pa×s	750.31	Joback Method
dvisc	0.0000485	Pa×s	818.18	Joback Method
dvisc	0.0000344	Pa×s	886.06	Joback Method
dvisc	0.0000256	Pa×s	953.93	Joback Method
dvisc	0.0000198	Pa×s	1021.80	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=U358732&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