Glutaric acid, 8-bromooctyl ethyl ester

Inchi: InChI=1S/C15H27BrO4/c1-2-19-14(17)10-9-11-15(18)20-13-8-6-4-3-5-7-12-16/h2-13H2,
InchiKey: BLQIWUUYEFGINR-UHFFFAOYSA-N
Formula: C15H27BrO4
SMILES: CCOC(=O)CCCC(=O)OCCCCCCCCBr
Mol. weight [g/mol]: 351.28

Physical Properties

Property code	Value	Unit	Source
gf	-378.10	kJ/mol	Joback Method
hf	-816.20	kJ/mol	Joback Method
hfus	45.46	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.998		Crippen Method
mcvol	254.590	ml/mol	McGowan Method
pc	1603.85	kPa	Joback Method
rinpol	2317.00		NIST Webbook
rinpol	2317.00		NIST Webbook
tb	761.34	K	Joback Method
tc	948.45	K	Joback Method
tf	462.93	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.51	J/mol×K	761.34	Joback Method
cpg	738.46	J/mol×K	792.53	Joback Method
cpg	752.57	J/mol×K	823.71	Joback Method
cpg	765.86	J/mol×K	854.90	Joback Method
cpg	778.35	J/mol×K	886.08	Joback Method
cpg	790.04	J/mol×K	917.27	Joback Method
cpg	800.95	J/mol×K	948.45	Joback Method
dvisc	0.0008853	Pa×s	462.93	Joback Method

dvisc	0.0004981	Pa×s	512.66	Joback Method
dvisc	0.0003103	Pa×s	562.40	Joback Method
dvisc	0.0002087	Pa×s	612.13	Joback Method
dvisc	0.0001490	Pa×s	661.87	Joback Method
dvisc	0.0001115	Pa×s	711.61	Joback Method
dvisc	0.0000867	Pa×s	761.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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