Glutaric acid, di(8-bromooctyl) ester

Inchi: InChI=1S/C21H38Br2O4/c22-16-9-5-1-3-7-11-18-26-20(24)14-13-15-21(25)27-19-12-8-4-2-6-10-17-23
InchiKey: VOONSKXYGYYGGU-UHFFFAOYSA-N
Formula: C21H38Br2O4
SMILES: O=C(CCCC(=O)OCCCCCCCCBr)OCCCCCCCCBr
Mol. weight [g/mol]: 514.33

Physical Properties

Property code	Value	Unit	Source
gf	-313.26	kJ/mol	Joback Method
hf	-913.71	kJ/mol	Joback Method
hfus	66.29	kJ/mol	Joback Method
hvap	93.52	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	6.714		Crippen Method
mcvol	356.630	ml/mol	McGowan Method
pc	1108.15	kPa	Joback Method
rinpol	3356.00		NIST Webbook
tb	964.78	K	Joback Method
tc	1181.40	K	Joback Method
tf	590.35	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1120.32	J/mol×K	964.78	Joback Method
cpg	1136.30	J/mol×K	1000.88	Joback Method
cpg	1151.07	J/mol×K	1036.99	Joback Method
cpg	1164.68	J/mol×K	1073.09	Joback Method
cpg	1177.18	J/mol×K	1109.19	Joback Method
cpg	1188.63	J/mol×K	1145.30	Joback Method
cpg	1199.07	J/mol×K	1181.40	Joback Method
dvisc	0.0002746	Pa×s	590.35	Joback Method
dvisc	0.0001534	Pa×s	652.75	Joback Method

dvisc	0.0000949	Pa×s	715.16	Joback Method
dvisc	0.0000634	Pa×s	777.57	Joback Method
dvisc	0.0000450	Pa×s	839.97	Joback Method
dvisc	0.0000335	Pa×s	902.38	Joback Method
dvisc	0.0000259	Pa×s	964.78	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U377244&Units=SI

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