Glutaric acid, 7-bromoheptyl pentyl ester

Inchi: InChI=1S/C17H31BrO4/c1-2-3-8-14-21-16(19)11-10-12-17(20)22-15-9-6-4-5-7-13-18/h2-
InchiKey: YUQCILOGAYBLPI-UHFFFAOYSA-N
Formula: C17H31BrO4
SMILES: CCCCCOC(=O)CCCC(=O)OCCCCCCCBr
Mol. weight [g/mol]: 379.33

Physical Properties

Property code	Value	Unit	Source
gf	-361.26	kJ/mol	Joback Method
hf	-857.48	kJ/mol	Joback Method
hfus	50.64	kJ/mol	Joback Method
hvap	78.18	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.779		Crippen Method
mcvol	282.770	ml/mol	McGowan Method
pc	1382.99	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	807.10	K	Joback Method
tc	996.10	K	Joback Method
tf	485.47	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.33	J/mol×K	807.10	Joback Method
cpg	907.87	J/mol×K	964.60	Joback Method
cpg	895.75	J/mol×K	933.10	Joback Method
cpg	882.75	J/mol×K	901.60	Joback Method
cpg	868.86	J/mol×K	870.10	Joback Method
cpg	854.05	J/mol×K	838.60	Joback Method
cpg	919.15	J/mol×K	996.10	Joback Method
dvisc	0.0000647	Pa×s	807.10	Joback Method

dvisc	0.0000838	Pa×s	753.50	Joback Method
dvisc	0.0001129	Pa×s	699.89	Joback Method
dvisc	0.0001599	Pa×s	646.28	Joback Method
dvisc	0.0002410	Pa×s	592.68	Joback Method
dvisc	0.0003942	Pa×s	539.07	Joback Method
dvisc	0.0007187	Pa×s	485.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380503&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