Glutaric acid, 7-bromoheptyl isobutyl ester

Inchi: InChI=1S/C16H29BrO4/c1-14(2)13-21-16(19)10-8-9-15(18)20-12-7-5-3-4-6-11-17/h14H,
InchiKey: JVXRPAZHYNNTMX-UHFFFAOYSA-N
Formula: C16H29BrO4
SMILES: CC(C)COC(=O)CCCC(=O)OCCCCCCCBr
Mol. weight [g/mol]: 365.30

Physical Properties

Property code	Value	Unit	Source
gf	-372.12	kJ/mol	Joback Method
hf	-842.12	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.245		Crippen Method
mcvol	268.680	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	783.78	K	Joback Method
tc	973.23	K	Joback Method
tf	459.20	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	780.96	J/mol×K	783.78	Joback Method
cpg	796.45	J/mol×K	815.36	Joback Method
cpg	811.03	J/mol×K	846.93	Joback Method
cpg	824.73	J/mol×K	878.51	Joback Method
cpg	837.55	J/mol×K	910.08	Joback Method
cpg	849.52	J/mol×K	941.66	Joback Method
cpg	860.65	J/mol×K	973.23	Joback Method
dvisc	0.0009230	Pa×s	459.20	Joback Method

dvisc	0.0004770	Pa×s	513.30	Joback Method
dvisc	0.0002796	Pa×s	567.39	Joback Method
dvisc	0.0001798	Pa×s	621.49	Joback Method
dvisc	0.0001242	Pa×s	675.59	Joback Method
dvisc	0.0000906	Pa×s	729.68	Joback Method
dvisc	0.0000690	Pa×s	783.78	Joback Method

Sources

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=U380501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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