

Glutaric acid, di(7-bromoheptyl) ester

Inchi: InChI=1S/C19H34Br2O4/c20-14-7-3-1-5-9-16-24-18(22)12-11-13-19(23)25-17-10-6-2-4-1
InchiKey: PTYYYNBYGLSVSU-UHFFFAOYSA-N
Formula: C19H34Br2O4
SMILES: O=C(CCCC(=O)OCCCCCBr)OCCCCCBr
Mol. weight [g/mol]: 486.28

Physical Properties

Property code	Value	Unit	Source
gf	-330.10	kJ/mol	Joback Method
hf	-872.43	kJ/mol	Joback Method
hfus	61.11	kJ/mol	Joback Method
hvap	89.07	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	5.934		Crippen Method
mvol	328.450	ml/mol	McGowan Method
pc	1264.65	kPa	Joback Method
rinpol	3053.00		NIST Webbook
rinpol	3053.00		NIST Webbook
tb	919.02	K	Joback Method
tc	1126.00	K	Joback Method
tf	567.81	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.87	J/molxK	919.02	Joback Method
cpg	1014.01	J/molxK	953.52	Joback Method
cpg	1028.09	J/molxK	988.01	Joback Method
cpg	1041.14	J/molxK	1022.51	Joback Method
cpg	1053.19	J/molxK	1057.01	Joback Method
cpg	1064.30	J/molxK	1091.50	Joback Method
cpg	1074.48	J/molxK	1126.00	Joback Method
dvisc	0.0003532	Paxs	567.81	Joback Method

dvisc	0.0002017	Paxs	626.35	Joback Method
dvisc	0.0001267	Paxs	684.88	Joback Method
dvisc	0.0000857	Paxs	743.41	Joback Method
dvisc	0.0000613	Paxs	801.95	Joback Method
dvisc	0.0000459	Paxs	860.49	Joback Method
dvisc	0.0000357	Paxs	919.02	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=U380505&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

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