

Glutaric acid, 7-bromoheptyl ethyl ester

Inchi: InChI=1S/C14H25BrO4/c1-2-18-13(16)9-8-10-14(17)19-12-7-5-3-4-6-11-15/h2-12H2,1H3
InchiKey: ASRLXJMQWYBHOP-UHFFFAOYSA-N
Formula: C14H25BrO4
SMILES: CCOC(=O)CCCC(=O)OCCCCCBr
Mol. weight [g/mol]: 337.25

Physical Properties

Property code	Value	Unit	Source
gf	-386.52	kJ/mol	Joback Method
hf	-795.56	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.608		Crippen Method
mvol	240.500	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	2454.00		NIST Webbook
rinpol	2454.00		NIST Webbook
tb	738.46	K	Joback Method
tc	925.54	K	Joback Method
tf	451.66	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.63	J/molxK	738.46	Joback Method
cpg	732.47	J/molxK	894.36	Joback Method
cpg	721.04	J/molxK	863.18	Joback Method
cpg	708.85	J/molxK	832.00	Joback Method
cpg	695.90	J/molxK	800.82	Joback Method
cpg	682.16	J/molxK	769.64	Joback Method
cpg	743.15	J/molxK	925.54	Joback Method
dvisc	0.0001000	Paxs	738.46	Joback Method

dvisc	0.0001282	Paxs	690.66	Joback Method
dvisc	0.0001705	Paxs	642.86	Joback Method
dvisc	0.0002374	Paxs	595.06	Joback Method
dvisc	0.0003503	Paxs	547.26	Joback Method
dvisc	0.0005568	Paxs	499.46	Joback Method
dvisc	0.0009762	Paxs	451.66	Joback Method

Sources

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=U380500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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