

Glutaric acid, 8-bromooctyl isobutyl ester

Inchi: InChI=1S/C17H31BrO4/c1-15(2)14-22-17(20)11-9-10-16(19)21-13-8-6-4-3-5-7-12-18/h1
InchiKey: KRVYWJZRAYMITD-UHFFFAOYSA-N
Formula: C17H31BrO4
SMILES: CC(C)COC(=O)CCCC(=O)OCCCCCCCCBr
Mol. weight [g/mol]: 379.33

Physical Properties

Property code	Value	Unit	Source
gf	-363.70	kJ/mol	Joback Method
hf	-862.76	kJ/mol	Joback Method
hfus	47.12	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	4.635		Crippen Method
mcvol	282.770	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	806.66	K	Joback Method
tc	997.07	K	Joback Method
tf	470.47	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.85	J/molxK	806.66	Joback Method
cpg	854.69	J/molxK	838.40	Joback Method
cpg	869.59	J/molxK	870.13	Joback Method
cpg	883.55	J/molxK	901.87	Joback Method
cpg	896.60	J/molxK	933.60	Joback Method
cpg	908.75	J/molxK	965.34	Joback Method
cpg	920.03	J/molxK	997.07	Joback Method
dvisc	0.0008259	Paxs	470.47	Joback Method

dvisc	0.0004218	Paxs	526.50	Joback Method
dvisc	0.0002452	Paxs	582.53	Joback Method
dvisc	0.0001567	Paxs	638.56	Joback Method
dvisc	0.0001077	Paxs	694.60	Joback Method
dvisc	0.0000783	Paxs	750.63	Joback Method
dvisc	0.0000595	Paxs	806.66	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=U377242&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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