

Glutaric acid, 4-bromophenyl isoheptyl ester

Inchi:	InChI=1S/C17H23BrO4/c1-13(2)5-4-12-21-16(19)6-3-7-17(20)22-15-10-8-14(18)9-11-15
InchiKey:	OGELGBDFULALOF-UHFFFAOYSA-N
Formula:	C17H23BrO4
SMILES:	CC(C)CCCOC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	371.27

Physical Properties

Property code	Value	Unit	Source
gf	-260.92	kJ/mol	Joback Method
hf	-637.70	kJ/mol	Joback Method
hfus	40.77	kJ/mol	Joback Method
hvap	80.73	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.504		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1787.88	kPa	Joback Method
rinpola	2488.00		NIST Webbook
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tb	838.32	K	Joback Method
tc	1051.65	K	Joback Method
tf	509.41	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.57	J/molxK	838.32	Joback Method
cpg	803.77	J/molxK	1016.09	Joback Method
cpg	793.97	J/molxK	980.54	Joback Method
cpg	783.18	J/molxK	944.98	Joback Method
cpg	771.36	J/molxK	909.43	Joback Method
cpg	758.50	J/molxK	873.87	Joback Method
cpg	812.60	J/molxK	1051.65	Joback Method
dvisc	0.0000612	Paxs	838.32	Joback Method

dvisc	0.0000782	Paxs	783.50	Joback Method
dvisc	0.0001039	Paxs	728.68	Joback Method
dvisc	0.0001444	Paxs	673.87	Joback Method
dvisc	0.0002129	Paxs	619.05	Joback Method
dvisc	0.0003384	Paxs	564.23	Joback Method
dvisc	0.0005943	Paxs	509.41	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=U358724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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