

Glutaric acid, 2,2-dichloroethyl 4-bromophenyl ester

Inchi:	InChI=1S/C13H13BrCl2O4/c14-9-4-6-10(7-5-9)20-13(18)3-1-2-12(17)19-8-11(15)16/h4-7
InchiKey:	YIAYPMNMJAFAY-UHFFFAOYSA-N
Formula:	C13H13BrCl2O4
SMILES:	O=C(CCCC(=O)Oc1ccc(Br)cc1)OCC(Cl)Cl
Mol. weight [g/mol]:	384.05

Physical Properties

Property code	Value	Unit	Source
gf	-318.46	kJ/mol	Joback Method
hf	-586.62	kJ/mol	Joback Method
hfus	38.81	kJ/mol	Joback Method
hvap	80.60	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.872		Crippen Method
mvol	227.130	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	2479.00		NIST Webbook
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tb	821.66	K	Joback Method
tc	1050.04	K	Joback Method
tf	524.17	K	Joback Method
vc	0.858	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.93	J/molxK	821.66	Joback Method
cpg	579.34	J/molxK	859.72	Joback Method
cpg	588.79	J/molxK	897.79	Joback Method
cpg	597.31	J/molxK	935.85	Joback Method
cpg	604.92	J/molxK	973.91	Joback Method
cpg	611.66	J/molxK	1011.97	Joback Method
cpg	617.53	J/molxK	1050.04	Joback Method
dvisc	0.0006025	Paxs	524.17	Joback Method

dvisc	0.0003724	Paxs	573.75	Joback Method
dvisc	0.0002485	Paxs	623.33	Joback Method
dvisc	0.0001760	Paxs	672.91	Joback Method
dvisc	0.0001307	Paxs	722.50	Joback Method
dvisc	0.0001008	Paxs	772.08	Joback Method
dvisc	0.0000803	Paxs	821.66	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U393289&Units=SI

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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