

Glutaric acid, di(2-(4-bromophenyl)ethyl) ester

Inchi:	InChI=1S/C21H22Br2O4/c22-18-8-4-16(5-9-18)12-14-26-20(24)2-1-3-21(25)27-15-13-17
InchiKey:	WGIZTGCIEMOFAQ-UHFFFAOYSA-N
Formula:	C21H22Br2O4
SMILES:	O=C(CCCC(=O)OCCc1ccc(Br)cc1)OCCc1ccc(Br)cc1
Mol. weight [g/mol]:	498.20

Physical Properties

Property code	Value	Unit	Source
gf	-107.70	kJ/mol	Joback Method
hf	-463.59	kJ/mol	Joback Method
hfus	53.59	kJ/mol	Joback Method
hvap	99.40	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	5.253		Crippen Method
mvol	309.110	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	3439.00		NIST Webbook
rinpol	3439.00		NIST Webbook
tb	1028.10	K	Joback Method
tc	1271.63	K	Joback Method
tf	668.23	K	Joback Method
vc	1.167	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.82	J/molxK	1028.10	Joback Method
cpg	911.38	J/molxK	1068.69	Joback Method
cpg	920.79	J/molxK	1109.28	Joback Method
cpg	929.11	J/molxK	1149.87	Joback Method
cpg	936.41	J/molxK	1190.45	Joback Method
cpg	942.78	J/molxK	1231.04	Joback Method
cpg	948.27	J/molxK	1271.63	Joback Method
dvisc	0.0001887	Paxs	668.23	Joback Method

dvisc	0.0001217	Paxs	728.21	Joback Method
dvisc	0.0000839	Paxs	788.19	Joback Method
dvisc	0.0000610	Paxs	848.16	Joback Method
dvisc	0.0000462	Paxs	908.14	Joback Method
dvisc	0.0000363	Paxs	968.12	Joback Method
dvisc	0.0000293	Paxs	1028.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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