

Glutaric acid, 2-ethylhexyl 4-bromophenyl ester

Inchi:	InChI=1S/C19H27BrO4/c1-3-5-7-15(4-2)14-23-18(21)8-6-9-19(22)24-17-12-10-16(20)11
InchiKey:	FULUOHQFIBPIQK-UHFFFAOYSA-N
Formula:	C19H27BrO4
SMILES:	CCCCC(CC)COC(=O)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	399.32

Physical Properties

Property code	Value	Unit	Source
gf	-244.08	kJ/mol	Joback Method
hf	-678.98	kJ/mol	Joback Method
hfus	45.95	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-6.17		Crippen Method
logp	5.284		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	2617.00		NIST Webbook
rinpol	2617.00		NIST Webbook
tb	884.08	K	Joback Method
tc	1096.44	K	Joback Method
tf	531.95	K	Joback Method
vc	1.095	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.87	J/molxK	884.08	Joback Method
cpg	920.50	J/molxK	1061.04	Joback Method
cpg	910.52	J/molxK	1025.65	Joback Method
cpg	899.50	J/molxK	990.26	Joback Method
cpg	887.40	J/molxK	954.87	Joback Method
cpg	874.21	J/molxK	919.47	Joback Method
cpg	929.47	J/molxK	1096.44	Joback Method
dvisc	0.0000456	Paxs	884.08	Joback Method

dvisc	0.0000586	Paxs	825.39	Joback Method
dvisc	0.0000785	Paxs	766.70	Joback Method
dvisc	0.0001102	Paxs	708.01	Joback Method
dvisc	0.0001646	Paxs	649.33	Joback Method
dvisc	0.0002661	Paxs	590.64	Joback Method
dvisc	0.0004785	Paxs	531.95	Joback Method

Sources

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=U393293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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