

Glutaric acid, naphth-2-ylmethyl 4-bromophenyl ester

Inchi:	InChI=1S/C22H19BrO4/c23-19-10-12-20(13-11-19)27-22(25)7-3-6-21(24)26-15-16-8-9-1
InchiKey:	MOZGBRKTMIELML-UHFFFAOYSA-N
Formula:	C22H19BrO4
SMILES:	O=C(CCCC(=O)Oc1ccc(Br)cc1)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	427.29

Physical Properties

Property code	Value	Unit	Source
gf	-6.95	kJ/mol	Joback Method
hf	-319.49	kJ/mol	Joback Method
hfus	47.92	kJ/mol	Joback Method
hvap	96.83	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	5.421		Crippen Method
mvol	286.240	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	3422.00		NIST Webbook
tb	1003.80	K	Joback Method
tc	1251.86	K	Joback Method
tf	652.40	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.61	J/molxK	1003.80	Joback Method
cpg	856.82	J/molxK	1045.14	Joback Method
cpg	867.01	J/molxK	1086.49	Joback Method
cpg	876.28	J/molxK	1127.83	Joback Method
cpg	884.73	J/molxK	1169.17	Joback Method
cpg	892.45	J/molxK	1210.51	Joback Method
cpg	899.56	J/molxK	1251.86	Joback Method
dvisc	0.0003683	Paxs	652.40	Joback Method
dvisc	0.0002499	Paxs	710.97	Joback Method

dvisc	0.0001799	Paxs	769.53	Joback Method
dvisc	0.0001357	Paxs	828.10	Joback Method
dvisc	0.0001062	Paxs	886.67	Joback Method
dvisc	0.0000857	Paxs	945.23	Joback Method
dvisc	0.0000709	Paxs	1003.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393301&Units=SI
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

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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