

Glutaric acid, 3-bromobenzyl 2-methylhex-3-yl ester

Inchi:	InChI=1S/C19H27BrO4/c1-4-7-17(14(2)3)24-19(22)11-6-10-18(21)23-13-15-8-5-9-16(20)
InchiKey:	CXPQZBHXXZELEQ-UHFFFAOYSA-N
Formula:	C19H27BrO4
SMILES:	CCCC(OC(=O)CCCC(=O)OCc1cccc(Br)c1)C(C)C
Mol. weight [g/mol]:	399.32

Physical Properties

Property code	Value	Unit	Source
gf	-246.52	kJ/mol	Joback Method
hf	-684.26	kJ/mol	Joback Method
hfus	42.43	kJ/mol	Joback Method
hvap	84.80	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.030		Crippen Method
mcvol	287.190	ml/mol	McGowan Method
pc	1539.08	kPa	Joback Method
rinpol	2807.00		NIST Webbook
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tb	883.64	K	Joback Method
tc	1098.00	K	Joback Method
tf	516.95	K	Joback Method
vc	1.089	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.39	J/molxK	883.64	Joback Method
cpg	921.22	J/molxK	1062.27	Joback Method
cpg	911.27	J/molxK	1026.55	Joback Method
cpg	900.24	J/molxK	990.82	Joback Method
cpg	888.10	J/molxK	955.09	Joback Method
cpg	874.83	J/molxK	919.37	Joback Method
cpg	930.14	J/molxK	1098.00	Joback Method
dvisc	0.0000417	Paxs	883.64	Joback Method

dvisc	0.0000544	Paxs	822.52	Joback Method
dvisc	0.0000742	Paxs	761.41	Joback Method
dvisc	0.0001068	Paxs	700.30	Joback Method
dvisc	0.0001649	Paxs	639.18	Joback Method
dvisc	0.0002789	Paxs	578.07	Joback Method
dvisc	0.0005344	Paxs	516.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377752&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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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