

Glutaric acid, 2-(3-bromophenyl)ethyl dodecyl ester

Inchi:	InChI=1S/C25H39BrO4/c1-2-3-4-5-6-7-8-9-10-11-19-29-24(27)16-13-17-25(28)30-20-18
InchiKey:	MYWCHMJLELLJHV-UHFFFAOYSA-N
Formula:	C25H39BrO4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCCc1cccc(Br)c1
Mol. weight [g/mol]:	483.48

Physical Properties

Property code	Value	Unit	Source
gf	-191.12	kJ/mol	Joback Method
hf	-797.54	kJ/mol	Joback Method
hfus	65.02	kJ/mol	Joback Method
hvap	98.93	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.169		Crippen Method
mvol	371.730	ml/mol	McGowan Method
pc	1013.59	kPa	Joback Method
rinpol	3337.00		NIST Webbook
rinpol	3337.00		NIST Webbook
tb	1021.80	K	Joback Method
tc	1251.48	K	Joback Method
tf	614.57	K	Joback Method
vc	1.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1221.24	J/molxK	1021.80	Joback Method
cpg	1236.89	J/molxK	1060.08	Joback Method
cpg	1251.09	J/molxK	1098.36	Joback Method
cpg	1263.89	J/molxK	1136.64	Joback Method
cpg	1275.36	J/molxK	1174.92	Joback Method
cpg	1285.57	J/molxK	1213.20	Joback Method
cpg	1294.58	J/molxK	1251.48	Joback Method
dvisc	0.0002140	Paxs	614.57	Joback Method

dvisc	0.0001182	Paxs	682.44	Joback Method
dvisc	0.0000727	Paxs	750.31	Joback Method
dvisc	0.0000485	Paxs	818.18	Joback Method
dvisc	0.0000344	Paxs	886.06	Joback Method
dvisc	0.0000256	Paxs	953.93	Joback Method
dvisc	0.0000198	Paxs	1021.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377215&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

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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