

Glutaric acid, dodecyl 5-methoxy-3-phenylpentyl ester

Inchi:	InChI=1S/C29H48O5/c1-3-4-5-6-7-8-9-10-11-15-23-33-28(30)19-16-20-29(31)34-25-22-2
InchiKey:	FDDSXXCCYGIGLO-UHFFFAOYSA-N
Formula:	C29H48O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCCC(CCOC)c1ccccc1
Mol. weight [g/mol]:	476.69

Physical Properties

Property code	Value	Unit	Source
gf	-269.57	kJ/mol	Joback Method
hf	-1032.46	kJ/mol	Joback Method
hfus	68.15	kJ/mol	Joback Method
hvap	102.76	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.374		Crippen Method
mcvol	416.460	ml/mol	McGowan Method
pc	776.77	kPa	Joback Method
rinqol	3439.00		NIST Webbook
tb	1064.16	K	Joback Method
tc	1314.18	K	Joback Method
tf	594.56	K	Joback Method
vc	1.611	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1462.49	J/molxK	1064.16	Joback Method
cpg	1528.95	J/molxK	1272.51	Joback Method
cpg	1519.74	J/molxK	1230.84	Joback Method
cpg	1508.57	J/molxK	1189.17	Joback Method
cpg	1495.35	J/molxK	1147.50	Joback Method
cpg	1480.02	J/molxK	1105.83	Joback Method
cpg	1536.27	J/molxK	1314.18	Joback Method
dvisc	0.0000092	Paxs	1064.16	Joback Method
dvisc	0.0000124	Paxs	985.89	Joback Method

dvisc	0.0000176	Paxs	907.63	Joback Method
dvisc	0.0000266	Paxs	829.36	Joback Method
dvisc	0.0000437	Paxs	751.09	Joback Method
dvisc	0.0000809	Paxs	672.83	Joback Method
dvisc	0.0001760	Paxs	594.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359538&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

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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