

Glutaric acid, 3-methoxybenzyl pentadecyl ester

Inchi:	InChI=1S/C28H46O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-22-32-27(29)20-17-21-28(30)31
InchiKey:	YXXVKYRKVXMGX-UHFFFAOYSA-N
Formula:	C28H46O5
SMILES:	CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1cccc(OC)c1
Mol. weight [g/mol]:	462.66

Physical Properties

Property code	Value	Unit	Source
gf	-285.18	kJ/mol	Joback Method
hf	-1018.01	kJ/mol	Joback Method
hfus	68.69	kJ/mol	Joback Method
hvap	101.58	kJ/mol	Joback Method
log10ws	-8.57		Crippen Method
logp	7.543		Crippen Method
mvol	402.370	ml/mol	McGowan Method
pc	809.37	kPa	Joback Method
rinpol	3458.00		NIST Webbook
rinpol	3458.00		NIST Webbook
tb	1046.70	K	Joback Method
tc	1290.03	K	Joback Method
tf	610.81	K	Joback Method
vc	1.562	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1398.39	J/molxK	1046.70	Joback Method
cpg	1464.35	J/molxK	1249.48	Joback Method
cpg	1455.12	J/molxK	1208.92	Joback Method
cpg	1443.96	J/molxK	1168.37	Joback Method
cpg	1430.83	J/molxK	1127.81	Joback Method
cpg	1415.66	J/molxK	1087.26	Joback Method
cpg	1471.71	J/molxK	1290.03	Joback Method
dvisc	0.0000123	Paxs	1046.70	Joback Method

dvisc	0.0000161	Paxs	974.05	Joback Method
dvisc	0.0000220	Paxs	901.40	Joback Method
dvisc	0.0000318	Paxs	828.75	Joback Method
dvisc	0.0000493	Paxs	756.11	Joback Method
dvisc	0.0000840	Paxs	683.46	Joback Method
dvisc	0.0001623	Paxs	610.81	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=U377200&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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