

Glutaric acid, naphth-2-ylmethyl 5-methyl-2-methoxybenzyl ester

Inchi:	InChI=1S/C24H24O5/c1-17-10-13-21(27-2)22(14-17)29-24(26)9-5-8-23(25)28-16-18-11-
InchiKey:	OZFVOIKMZOIJDR-UHFFFAOYSA-N
Formula:	C24H24O5
SMILES:	COc1ccc(C)cc1OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	392.44

Physical Properties

Property code	Value	Unit	Source
gf	-119.06	kJ/mol	Joback Method
hf	-530.79	kJ/mol	Joback Method
hfus	48.61	kJ/mol	Joback Method
hvap	97.92	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	4.976		Crippen Method
mcvol	302.790	ml/mol	McGowan Method
pc	1496.51	kPa	Joback Method
rinqol	3346.00		NIST Webbook
tb	1010.80	K	Joback Method
tc	1248.42	K	Joback Method
tf	649.89	K	Joback Method
vc	1.151	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	957.58	J/molxK	1010.80	Joback Method
cpg	969.44	J/molxK	1050.40	Joback Method
cpg	979.93	J/molxK	1090.01	Joback Method
cpg	989.10	J/molxK	1129.61	Joback Method
cpg	997.00	J/molxK	1169.21	Joback Method
cpg	1003.70	J/molxK	1208.81	Joback Method
cpg	1009.24	J/molxK	1248.42	Joback Method
dvisc	0.0002788	Paxs	649.89	Joback Method
dvisc	0.0001875	Paxs	710.04	Joback Method

dvisc	0.0001341	Paxs	770.19	Joback Method
dvisc	0.0001007	Paxs	830.35	Joback Method
dvisc	0.0000786	Paxs	890.50	Joback Method
dvisc	0.0000633	Paxs	950.65	Joback Method
dvisc	0.0000523	Paxs	1010.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393935&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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