

Glutaric acid, naphth-2-ylmethyl 2-isopropoxyphenyl ester

Inchi:	InChI=1S/C25H26O5/c1-18(2)29-22-10-5-6-11-23(22)30-25(27)13-7-12-24(26)28-17-19-
InchiKey:	KXCPNAZEFRRRTAY-UHFFFAOYSA-N
Formula:	C25H26O5
SMILES:	CC(C)Oc1ccccc1OC(=O)CCCC(=O)OCc1ccc2ccccc2c1
Mol. weight [g/mol]:	406.47

Physical Properties

Property code	Value	Unit	Source
gf	-103.45	kJ/mol	Joback Method
hf	-545.24	kJ/mol	Joback Method
hfus	48.07	kJ/mol	Joback Method
hvap	99.09	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	5.446		Crippen Method
mcvol	316.880	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
tb	1028.26	K	Joback Method
tc	1267.42	K	Joback Method
tf	633.64	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1018.71	J/molxK	1028.26	Joback Method
cpg	1030.77	J/molxK	1068.12	Joback Method
cpg	1041.45	J/molxK	1107.98	Joback Method
cpg	1050.80	J/molxK	1147.84	Joback Method
cpg	1058.89	J/molxK	1187.70	Joback Method
cpg	1065.80	J/molxK	1227.56	Joback Method
cpg	1071.60	J/molxK	1267.42	Joback Method
dvisc	0.0002837	Paxs	633.64	Joback Method
dvisc	0.0001757	Paxs	699.41	Joback Method
dvisc	0.0001182	Paxs	765.18	Joback Method

dvisc	0.0000846	Paxs	830.95	Joback Method
dvisc	0.0000637	Paxs	896.72	Joback Method
dvisc	0.0000498	Paxs	962.49	Joback Method
dvisc	0.0000402	Paxs	1028.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391879&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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