

Glutaric acid, 2-methylhex-3-yl 2-phenoxyethyl ester

Inchi:	InChI=1S/C20H30O5/c1-4-9-18(16(2)3)25-20(22)13-8-12-19(21)24-15-14-23-17-10-6-5-7
InchiKey:	IQYMFQDNIURTHI-UHFFFAOYSA-N
Formula:	C20H30O5
SMILES:	CCCC(OC(=O)CCCC(=O)OCCOc1ccccc1)C(C)C
Mol. weight [g/mol]:	350.45

Physical Properties

Property code	Value	Unit	Source
gf	-347.79	kJ/mol	Joback Method
hf	-851.98	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	82.34	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.147		Crippen Method
mcvol	289.650	ml/mol	McGowan Method
pc	1355.63	kPa	Joback Method
rinpola	2453.00		NIST Webbook
tb	857.80	K	Joback Method
tc	1061.53	K	Joback Method
tf	478.13	K	Joback Method
vc	1.101	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.81	J/molxK	857.80	Joback Method
cpg	976.07	J/molxK	1027.57	Joback Method
cpg	965.08	J/molxK	993.62	Joback Method
cpg	952.87	J/molxK	959.66	Joback Method
cpg	939.44	J/molxK	925.71	Joback Method
cpg	924.76	J/molxK	891.75	Joback Method
cpg	985.87	J/molxK	1061.53	Joback Method
dvisc	0.0000340	Paxs	857.80	Joback Method
dvisc	0.0000456	Paxs	794.52	Joback Method

dvisc	0.0000643	Paxs	731.24	Joback Method
dvisc	0.0000969	Paxs	667.96	Joback Method
dvisc	0.0001590	Paxs	604.69	Joback Method
dvisc	0.0002929	Paxs	541.41	Joback Method
dvisc	0.0006344	Paxs	478.13	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376917&Units=SI

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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