

Glutaric acid, 3-methylbut-2-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H28O5/c1-17(2)18(3)27-23(25)14-8-13-22(24)26-16-19-9-7-12-21(15-19)2

InchiKey: PXSCXNJMPNKGLR-UHFFFAOYSA-N

Formula: C23H28O5

SMILES: CC(C)C(C)OC(=O)CCCC(=O)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 384.47

Physical Properties

Property code	Value	Unit	Source
gf	-219.75	kJ/mol	Joback Method
hf	-688.84	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	91.95	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.280		Crippen Method
mcvol	308.160	ml/mol	McGowan Method
pc	1384.02	kPa	Joback Method
rinpol	2827.00		NIST Webbook
rinpol	2827.00		NIST Webbook
tb	958.10	K	Joback Method
tc	1184.39	K	Joback Method
tf	550.88	K	Joback Method
vc	1.161	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.42	J/molxK	958.10	Joback Method
cpg	999.03	J/molxK	995.82	Joback Method
cpg	1011.09	J/molxK	1033.53	Joback Method
cpg	1021.63	J/molxK	1071.25	Joback Method
cpg	1030.70	J/molxK	1108.96	Joback Method
cpg	1038.31	J/molxK	1146.68	Joback Method
cpg	1044.51	J/molxK	1184.39	Joback Method
dvisc	0.0003191	Paxs	550.88	Joback Method

dvisc	0.0001613	Paxs	618.75	Joback Method
dvisc	0.0000933	Paxs	686.62	Joback Method
dvisc	0.0000596	Paxs	754.49	Joback Method
dvisc	0.0000410	Paxs	822.36	Joback Method
dvisc	0.0000298	Paxs	890.23	Joback Method
dvisc	0.0000227	Paxs	958.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392123&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
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
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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