Fumaric acid, 2,4,4-trimethylpentyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C23H28O4/c1-17(14-23(2,3)4)15-26-21(24)11-12-22(25)27-16-18-9-10-19-7-5-

InchiKey: OMKYRCZPQCDXDZ-VAWYXSNFSA-N

Formula: C23H28O4

SMILES: CC(COC(=O)C=CC(=O)OCc1ccc2ccccc2c1)CC(C)(C)C

Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-35.01	kJ/mol	Joback Method
hf	-488.33	kJ/mol	Joback Method
hfus	40.84	kJ/mol	Joback Method
hvap	87.96	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.055		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1377.86	kPa	Joback Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		NIST Webbook
tb	929.35	K	Joback Method
tc	1155.08	K	Joback Method
tf	547.27	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.40	J/mol×K	929.35	Joback Method
cpg	967.56	J/mol×K	966.97	Joback Method
cpg	981.71	J/mol×K	1004.59	Joback Method
cpg	994.96	J/mol×K	1042.22	Joback Method
cpg	1007.43	J/mol×K	1079.84	Joback Method
cpg	1019.21	J/mol×K	1117.46	Joback Method
cpg	1030.41	J/mol×K	1155.08	Joback Method
dvisc	0.0004778	Pa×s	547.27	Joback Method

dvisc	0.0002621	Pa×s	610.95	Joback Method
dvisc	0.0001611	Pa×s	674.63	Joback Method
dvisc	0.0001077	Pa×s	738.31	Joback Method
dvisc	0.0000767	Pa×s	801.99	Joback Method
dvisc	0.0000574	Pa×s	865.67	Joback Method
dvisc	0.0000448	Pa×s	929.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405616&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

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