Fumaric acid, 3-methylbutyl naphth-2-ylmethyl ester

Inchi: InChI=1S/C20H22O4/c1-15(2)11-12-23-19(21)9-10-20(22)24-14-16-7-8-17-5-3-4-6-18(17

InchiKey: DZHVXGKFJFWGQK-MDZDMXLPSA-N

Formula: C20H22O4

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

Mol. weight [g/mol]: 326.39

Physical Properties

Property code	Value	Unit	Source
gf	-63.11	kJ/mol	Joback Method
hf	-417.66	kJ/mol	Joback Method
hfus	40.48	kJ/mol	Joback Method
hvap	82.57	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.029		Crippen Method
mcvol	260.020	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2637.00		NIST Webbook
rinpol	2637.00		NIST Webbook
tb	863.94	K	Joback Method
tc	1085.85	K	Joback Method
tf	511.04	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	776.26	J/mol×K	863.94	Joback Method
cpg	790.51	J/mol×K	900.92	Joback Method
cpg	803.73	J/mol×K	937.91	Joback Method
cpg	815.99	J/mol×K	974.89	Joback Method
cpg	827.35	J/mol×K	1011.88	Joback Method
cpg	837.89	J/mol×K	1048.86	Joback Method
cpg	847.67	J/mol×K	1085.85	Joback Method
dvisc	0.0007089	Pa×s	511.04	Joback Method

dvisc	0.0004169	Pa×s	569.86	Joback Method
dvisc	0.0002708	Pa×s	628.67	Joback Method
dvisc	0.0001893	Pa×s	687.49	Joback Method
dvisc	0.0001401	Pa×s	746.31	Joback Method
dvisc	0.0001083	Pa×s	805.12	Joback Method
dvisc	0.0000867	Pa×s	863.94	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=U405557&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